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Abstract

Despite the growing popularity of diagnostic classification models (e.g., Rupp, Templin, & Henson, 2010) in educational and psychological measurement, methods for testing their absolute goodness-of-fit to real data remain relatively underdeveloped. For tests of reasonable length and for realistic sample size, full-information test statistics such as Pearson's X^2 and the likelihood ratio statistic G^2 suffer from sparseness in the underlying contingency table from which they are computed. Recently, limited-information fit statistics such as Maydeu-Olivares and Joe's (2006) M_2 have been found to be quite useful in testing the overall goodness-of-fit fit of item response theory (IRT) models. In this study, we applied Maydeu-Olivares and Joe's (2006) M_2 statistic to diagnostic classification models. Through a series of simulation studies, we found that M_2 is well calibrated across a wide range of diagnostic model structures and was sensitive to certain misspecifications of the item model (e.g., fitting disjunctive models to data generated according to a conjunctive model), errors in the Q-matrix (adding or omitting paths, omitting a latent variable), and violations of local item independence due to unmodeled testlet effects. On the other hand, M_2 was largely insensitive to misspecifications in the distribution of higher-order latent dimensions and to the specification of an extraneous attribute. To complement the analyses of the overall model goodness-of-fit using M_2, we investigated the utility of the Chen and Thissen (1997) local dependence statistic X_{LD}^2 for characterizing sources of misfit, an important aspect of model appraisal often overlooked in favor of overall statements. The X_{LD}^2 statistic was found to be slightly conservative (with Type I error rates consistently below the nominal level) but still useful in pinpointing the sources of misfit. Patterns of local dependence arising due to specific model misspecifications are illustrated. Finally, we used the M_2 and X_{LD}^2 statistics to evaluate a diagnostic model fit to data from the Trends in Mathematics and Science Study (TIMSS), drawing upon analyses previously conducted by Lee, Park, and Taylan (2011).

Keywords: diagnostic classification models, item response models, limited-information goodness-of-fit, local item independence

1 Introduction

Diagnostic classification models (see, e.g., Rupp, Templin, & Henson, 2010) have received increasing attention within the field of educational and psychological measurement. The popularity of these models may be largely due to their perceived ability to provide useful information concerning both examinees (classifying them according to their attribute profiles) and test items (describing the particular attributes that are relevant to or required in order to achieve a certain response). Despite these attractive features, it is important to note the potential for biased interpretations when such models are misspecified. Various authors have noted that methods for evaluating the fit of diagnostic models remain relatively underdeveloped (e.g., Maris & Bechger, 2009; Wilhelm & Robitzsch, 2009; Rupp et al., 2010). That said, there has been notable progress (e.g., Sinharay & Almond, 2009; Lai, Cui, & Gierl, 2012; de la Torre, 2008; Rupp & Templin, 2008; Kunina-Habenicht, Rupp, & Wilhelm, 2012).

In this study, we examine the utility of limited information goodness-of-fit statistics (e.g., Bartholomew & Leung, 2002) for evaluating the fit of diagnostic classification models. Specifically, we apply M_2, an overall test statistic proposed by Maydeu-Olivares & Joe (2006), to a range of diagnostic model structures and consider its calibration and sensitivity across a range of misspecifications. Various M_2-type statistics have been applied to an increasing assortment of item response theory (IRT) models (e.g., Cai, Maydeu-Olivares, Coffman, & Thissen, 2006; Joe & Maydeu-Olivares, 2010; Cai & Hansen, 2013; Cai & Monroe, 2014). Limited-information fit statistics have been suggested as a possible approach for evaluating the use of diagnostic models (e.g., Rupp et al., 2010), and initial applications appear quite promising (Templin, 2007; Jurich, Bradshaw, & DeMars, 2014). Here, we seek to continue to develop this line of work.

Additionally, we demonstrate how the use of Chen and Thissen's (1997) local dependence index, X^2_{LD}, can complement the application of M_2 in practice. While M_2 provides a test of the overall fit of the model, it does not pinpoint the source of any misfit. The X^2_{LD} index, on the other hand, evaluates the fit of the model to item pairs, and can be useful in identifying the source of misfit. As both M_2 and X^2_{LD} are based on marginal subtables (of the entire contingency table of possible response patterns), the use of X^2_{LD} following a significant M_2 test may be viewed as akin to the *post hoc* multiple comparison procedures routinely employed in linear models.

This research, then, can be viewed as an application of existing methodology to a new context: diagnostic classification models. Our goal is to evaluate the performance of limited-information statistics for testing the fit of diagnostic classification models, over a wide range of data generating conditions and kinds of model misspecification. While diagnostic classification models and standard IRT models are conceptually related, we should not assume that limited-information testing methodology will be equivalently useful for the two modeling frameworks. Instead, we view the utility of limited information testing for diagnostic classification models as an empirical question worthy of investigation. Moreover, there are features of diagnostic classification models, such as the so-called Q-matrix, with no analog in IRT. Thus, it is unknown whether limited-information test statistics are sensitive to misspecifications of these aspects. Finally, as part of this research effort, both M_2 and X_{LD}^2 have been implemented in a publicly available software distribution (Cai, 2015) to analyze misfit in diagnostic classification models, which should benefit practitioners, as well as other methodologists.

The rest of this manuscript is organized as follows. We begin by describing diagnostic modeling and the application of M_2 to this modeling context. Next, we evaluate the performance of M_2 and X_{LD}^2 through a series of simulation studies. We then illustrate how M_2 and X_{LD}^2 may be used in tandem to assess and revise a diagnostic model fit to real data. Finally, we discuss some of the limitations of this research and opportunities to further develop this work.

2 General Diagnostic Classification Modeling Framework

2.1 An Item Response Model for Diagnostic Classification

In this section, we describe a higher-order, hierarchical diagnostic classification model (Cai, 2013) to which we will apply the limited-information statistic. This model may be best understood as an extension of existing diagnostic modeling frameworks, such as the log-linear cognitive diagnosis model (LCDM; Henson, Templin, & Willse, 2009), which we use here as a starting point. Let there be a total of $i = 1, \ldots, I$ items. In this research we limit the scope to dichotomously scored items, noting that extending the theory to multiple-categorical data is straightforward. Let the response categories be coded as 0 (incorrect/no endorsement) or 1

(correct/endorsement). Let there be K dichotomous (0-1) underlying latent attribute variables, $\boldsymbol{x} = (x_1, \ldots, x_k, \ldots, x_K)'$, where $x_k = 1$ indicates mastery/possession of an attribute. The relationship between items and attributes is captured by the Q-matrix, which is an $I \times K$ matrix of zeros and ones. The (i, k)th entry in the Q-matrix is denoted as q_{ik}, and takes on a value of one if item i measures attribute k.

Let $T_i(1|\boldsymbol{x})$ be the category 1 response function for item i:

$$T_i(1|\boldsymbol{x}) = \frac{1}{1 + \exp(-\eta_i)}, \tag{1}$$

where the linear predictor is

$$\eta_i = \alpha_i + \boldsymbol{\lambda}_i' h_i(\mathbf{Q}, \boldsymbol{x}). \tag{2}$$

It follows that for category 0, the response function is

$$T_i(0|\boldsymbol{x}) = 1.0 - T_i(1|\boldsymbol{x}). \tag{3}$$

The αs and λs in the linear predictor are the item parameters, and $h_i(\mathbf{Q}, \boldsymbol{x})$ is a potentially vector-valued function that defines how the measured attributes combine to create the linear predictor portion of the item response model in Equation (2). As noted by Henson et al. (2009), placing certain constraints on the λs yields several of the more commonly utilized diagnostic models (see also Rupp et al., 2010; Choi, Rupp, & Pan, 2013). For instance, suppose that according to the Q-matrix, a mathematics test item i measures two particular algebra-related skills (attributes x_1 and x_2), and that successful solution of the item requires both. The linear predictor may take the following deterministic-input noisy "and" gate (DINA; Junker & Sijtsma, 2001) form, with a single free parameter for the interaction term:

$$\eta_i = \alpha_i + 0x_1 + 0x_2 + \lambda_i x_1 x_2. \tag{4}$$

In this case, $h_i(\mathbf{Q}, \boldsymbol{x}) = (x_1, x_2, x_1 x_2)'$ contains the main effects and the second-order interaction, and $\boldsymbol{\lambda}_i = (0, 0, \lambda_i)'$ contains fixed parameters. Alternatively, perhaps the item only requires the mastery of either attribute 1 or attribute 2. Then the linear predictor of the IRT model may take the following deterministic-input noisy "or" gate (DINO; Templin & Henson, 2006) form, with a single slope parameter set equal between the main effects and the interaction term in absolute magnitude, albeit the interaction term is of the opposite direction:

$$\eta_i = \alpha_i + \lambda_i x_1 + \lambda_i x_2 - \lambda_i x_1 x_2. \tag{5}$$

These constraints reflect the specification that mastery of both attributes does not lead to any further increase in the logit (beyond the effect of mastering of one of the attributes), and in this case $\boldsymbol{\lambda}_i = (\lambda_i, \lambda_i, -\lambda_i)'$ contains linear restrictions. Yet another possibility is that each attribute contributes to some increase in the logit, and that the magnitude of the increase due to one attribute does not depend on the mastery of the other. In that case, the linear predictor might contain only the main effect terms, and the model would take the form of von Davier's (2005) general diagnostic model or the compensatory reparameterized unified model (C-RUM; Hartz, 2002):

$$\eta_i = \alpha_i + \lambda_i x_1 + \lambda_i x_2. \tag{6}$$

Let Y_i be a random variable whose realization y_i is a response to item i. Regardless of the exact form of the model or the number of attributes, the probability mass function of Y_i, conditional on $\boldsymbol{x}$, is that of a Bernoulli:

$$P(Y_i = y_i|\boldsymbol{x}) = [T_i(y_i|\boldsymbol{x})]^{y_i}[1.0 - T_i(y_i|\boldsymbol{x})]^{1-y_i}. \tag{7}$$

2.2 Hierarchical and Higher-Order Extensions

Conditional independence is a critical assumption for model building in all of IRT analysis. In the case of DCMs, it is customary to assume the independence of item responses given the attributes (e.g., Templin & Henson, 2006). That is, the conditional response pattern probability factors:

$$\pi(\boldsymbol{y}|\boldsymbol{x}) = P\left(\cap_{i=1}^{I} Y_i = y_i \,\middle|\, \boldsymbol{x}\right) = \prod_{i=1}^{I} P(Y_i = y_i|\boldsymbol{x}), \tag{8}$$

where $\boldsymbol{y} = (y_1, \ldots, y_I)'$ is an $I \times 1$ vector that contains the observed response pattern. However, conditional independence may be unrealistic if item i belongs to a cluster of items dependent on the same stimulus (as in a passage-based reading assessment), or if this item falls into a specific content subdomain (e.g., social aspects of quality of life) along with some other items, or if it is part of a measure repeatedly administered to the same group of respondents (e.g., in longitudinal studies). A standard strategy in item factor analysis is to include additional random effects to account for potential residual dependence due to common sources of variation shared by subsets of items (Cai, Yang, & Hansen, 2011). Let there be S such clusters of

items, indexed $s = 1, \dots, S$. If we assume that the clusters are mutually exclusive and that each item is permitted to load on at most one specific dimension, then the response function for item i in category 1 becomes

$$T_i(1|\boldsymbol{x}, \xi_s) = \frac{1}{1 + \exp\left[-\left(\alpha_i + \boldsymbol{\lambda}_i' h_i(\mathbf{Q}, \boldsymbol{x}) + \beta_s \xi_s\right)\right]}, \tag{9}$$

where β_s is the item slope on specific factor/dimension ξ_s. Again the response function for category 0 becomes

$$T_i(0|\boldsymbol{x}, \xi_s) = 1.0 - T_i(1|\boldsymbol{x}, \xi_s). \tag{10}$$

The model resembles a bifactor model or testlet model (Gibbons & Hedeker, 1992). With the additional random effects, conditional independence may be more amenable:

$$\pi(\boldsymbol{y}|\boldsymbol{x}, \xi_1, \dots, \xi_S) = P\left(\cap_{i=1}^{I} Y_i = y_i \,\middle|\, \boldsymbol{x}, \xi_1, \dots, \xi_S\right) = \prod_{s=1}^{S} \prod_{i \in \mathfrak{H}_s} P(Y_i = y_i|\boldsymbol{x}, \xi_s), \tag{11}$$

where $\mathfrak{H}_s$ is a notational shorthand for the set of items that load on specific dimension s, and $P(Y_i = y_i|\boldsymbol{x}, \xi_s) = [T_i(y_i|\boldsymbol{x}, \xi_s)]^{y_i}[T_i(y_i|\boldsymbol{x}, \xi_s)]^{1-y_i}$ is again a Bernoulli probability mass function.

Suppose the distribution of the ξ's is given by $g(\xi_1|\boldsymbol{x})g(\xi_2|\boldsymbol{x}) \cdots g(\xi_S|\boldsymbol{x})$; that is, the specific dimensions are conditionally independent given $\boldsymbol{x}$. We may integrate all S specific dimensions out without a full S-dimensional integral. This is because we may utilize the familiar dimension reduction method (see Cai et al., 2011; Rijmen, 2009) developed for item bifactor analysis to transform the following S-fold integral

$$\pi(\boldsymbol{y}|\boldsymbol{x}) = \int \pi(\boldsymbol{y}|\boldsymbol{x}, \xi_1, \dots, \xi_S)\, g(\xi_1|\boldsymbol{x}) \cdots g(\xi_S|\boldsymbol{x}) d\xi_1 \cdots d\xi_S, \tag{12}$$

into a series of one-dimensional integrals

$$\begin{aligned} \pi(\boldsymbol{y}|\boldsymbol{x}) &= \int \prod_{s=1}^{S} \prod_{i \in \mathfrak{H}_s} P(Y_i = y_i|\boldsymbol{x}, \xi_s)\, g(\xi_1|\boldsymbol{x}) \cdots g(\xi_S|\boldsymbol{x}) d\xi_1 \cdots d\xi_S \\ &= \prod_{s=1}^{S} \int \prod_{i \in \mathfrak{H}_s} P(Y_i = y_i|\boldsymbol{x}, \xi_s)\, g(\xi_s|\boldsymbol{x}) d\xi_s, \end{aligned} \tag{13}$$

which will vastly reduce the amount of time needed for maximum marginal likelihood based parameter estimation because these integrals must be numerically evaluated.

As per de la Torre & Douglas (2004), we may further model the latent attribute profiles for individuals by regressing the xs on m higher-order dimensions $\boldsymbol{\theta}$. For example, we may use

a multidimensional extension of the 2-parameter logistic model (Reckase, 2009) to relate the latent attributes to the latent dimensions:

$$P(x_k = 1|\boldsymbol{\theta}) = \pi_k(\boldsymbol{\theta}) = \frac{1}{1 + \exp[-(a_{k0} + a_{k1}\theta_1 + \cdots + a_{km}\theta_m)]}. \quad (14)$$

Again, if we assume conditional independence of the latent attributes given $\boldsymbol{\theta}$, we may write

$$\pi(\boldsymbol{x}|\boldsymbol{\theta}) = \prod_{k=1}^{K} [\pi_k(\boldsymbol{\theta})]^{x_k}[1 - \pi_k(\boldsymbol{\theta})]^{1-x_k}. \quad (15)$$

When we combine $\pi(\boldsymbol{y}|\boldsymbol{x})$ from Equation (11) with $\pi(\boldsymbol{x}|\boldsymbol{\theta})$ from Equation (14), we see that the contribution to marginal likelihood from response pattern $\boldsymbol{y}$ can be obtained as:

$$\pi(\boldsymbol{y}) = \int \left[\int \pi(\boldsymbol{y}|\boldsymbol{x})\pi(\boldsymbol{x}|\boldsymbol{\theta})d\boldsymbol{x} \right] g(\boldsymbol{\theta})\, d\boldsymbol{\theta}, \quad (16)$$

where the integral in the brackets is actually a 2^K-term summation over the (conditional) attribute profile probabilities for all $\boldsymbol{x}$.

3 Limited-information Goodness-of-fit Testing

3.1 Maximum Marginal Likelihood Estimation

Let $\boldsymbol{\gamma}$ be a $d \times 1$ vector that collects together all free parameters in the model. These include parameters from all I items (the α's, β's, and λ's), parameters for the distribution of the specific dimensions $g(\xi_s|\boldsymbol{x})$, the higher-order IRT model (the a's), and the parameters from the distribution of the higher-order dimensions $g(\boldsymbol{\theta})$. To emphasize the fact that the marginal likelihood in Equation (16) is a function of the parameters once the response pattern is observed (and considered fixed), let $\pi_{\boldsymbol{y}}(\boldsymbol{\gamma})$ denote the marginal likelihood.

For I items, the IRT model generates a total of $C = 2^I$ cross-classifications or possible item response patterns in the form of a contingency table. Based on a sample of N respondents, let the observed proportion associated with pattern $\boldsymbol{y} = (y_1, \ldots, y_I)'$ be denoted as $p_{\boldsymbol{y}}$. The sampling model for this contingency table is a multinomial distribution with C cells and N trials. The multinomial log-likelihood for the item parameters $\boldsymbol{\gamma}$ is proportional to

$$\log L(\boldsymbol{\gamma}) \propto N \sum_{\boldsymbol{y}} p_{\boldsymbol{y}} \log \pi_{\boldsymbol{y}}(\boldsymbol{\gamma}), \quad (17)$$

where the summation is over all C response patterns. Maximization of the log-likelihood (e.g., with the EM algorithm; Bock & Aitkin, 1981) leads to the maximum marginal likelihood estimator $\widehat{\boldsymbol{\gamma}}$.

Upon finding $\widehat{\boldsymbol{\gamma}}$, the model generates model-implied probabilities for each response pattern $\hat{\pi}_{\boldsymbol{y}} = \pi_{\boldsymbol{y}}(\widehat{\boldsymbol{\gamma}})$. Suppose all the model-implied response pattern probabilities $\hat{\pi}_{\boldsymbol{y}}$ are collected into a $C \times 1$ vector $\widehat{\boldsymbol{\pi}}$. By analogy, let a $C \times 1$ vector $\boldsymbol{\pi}_*$ contain the true (population) response pattern probabilities. Similarly, all the observed proportions $p_{\boldsymbol{y}}$ can be collected into a $C \times 1$ vector $\boldsymbol{p}$. For example, for 3 items there are $2^3 = 8$ item response patterns, and the response pattern probabilities and observed proportions are:

$$\boldsymbol{\pi}_* = \begin{pmatrix} \pi_{000} \\ \pi_{001} \\ \pi_{010} \\ \pi_{011} \\ \pi_{100} \\ \pi_{101} \\ \pi_{110} \\ \pi_{111} \end{pmatrix}, \widehat{\boldsymbol{\pi}} = \begin{pmatrix} \hat{\pi}_{000} \\ \hat{\pi}_{001} \\ \hat{\pi}_{010} \\ \hat{\pi}_{011} \\ \hat{\pi}_{100} \\ \hat{\pi}_{101} \\ \hat{\pi}_{110} \\ \hat{\pi}_{111} \end{pmatrix} = \begin{pmatrix} \pi_{000}(\widehat{\boldsymbol{\gamma}}) \\ \pi_{001}(\widehat{\boldsymbol{\gamma}}) \\ \pi_{010}(\widehat{\boldsymbol{\gamma}}) \\ \pi_{011}(\widehat{\boldsymbol{\gamma}}) \\ \pi_{100}(\widehat{\boldsymbol{\gamma}}) \\ \pi_{101}(\widehat{\boldsymbol{\gamma}}) \\ \pi_{110}(\widehat{\boldsymbol{\gamma}}) \\ \pi_{111}(\widehat{\boldsymbol{\gamma}}) \end{pmatrix}, \boldsymbol{p} = \begin{pmatrix} p_{000} \\ p_{001} \\ p_{010} \\ p_{011} \\ p_{100} \\ p_{101} \\ p_{110} \\ p_{111} \end{pmatrix}. \quad (18)$$

Using this setup, exactly correct model specification (i.e., perfect model fit) in the population can be understood as the statement that there exists $\boldsymbol{\gamma}_*$ such that $\boldsymbol{\pi}(\boldsymbol{\gamma}_*) = \boldsymbol{\pi}_*$. The values $\boldsymbol{\gamma}_*$ may be taken as the true parameters to be estimated.

Under correct model specification, from results in discrete multivariate analysis (e.g., Bishop, Fienberg, & Holland, 1975), the maximum likelihood estimator is consistent, asymptotically normal and asymptotically efficient, which can be summarized as follows:

$$\sqrt{N}(\widehat{\boldsymbol{\gamma}} - \boldsymbol{\gamma}_*) \xrightarrow{D} \mathcal{N}_d(\mathbf{0}, \mathcal{F}^{-1}), \quad (19)$$

where $\mathcal{F} = \boldsymbol{\Delta}_*' \, [diag(\boldsymbol{\pi}_*)]^{-1} \boldsymbol{\Delta}_*$ is the $d \times d$ Fisher information matrix, with the Jacobian matrix $\boldsymbol{\Delta}_*$ defined as the $C \times d$ matrix of all first-order partial derivatives of the response pattern probabilities with respect to the parameters, evaluated at $\boldsymbol{\gamma}_*$:

$$\boldsymbol{\Delta}_* = \frac{\partial \boldsymbol{\pi}(\boldsymbol{\gamma}_*)}{\partial \boldsymbol{\gamma}'}.$$

3.2 Distribution of Residuals under Maximum Likelihood Estimation

It can be shown (e.g., Bishop et al., 1975) that the asymptotic distribution of $(\boldsymbol{p} - \boldsymbol{\pi}_*)$ is C-variate normal:

$$\sqrt{N}(\boldsymbol{p} - \boldsymbol{\pi}_*) \xrightarrow{D} \mathcal{N}_C(\mathbf{0}, \Xi), \tag{20}$$

where $\Xi = diag(\boldsymbol{\pi}_*) - \boldsymbol{\pi}_*\boldsymbol{\pi}_*'$ is the multinomial covariance matrix. Under maximum likelihood estimation, the cell residual vector $(\boldsymbol{p} - \hat{\boldsymbol{\pi}})$ is asymptotically C-variate normal:

$$\sqrt{N}(\boldsymbol{p} - \hat{\boldsymbol{\pi}}) \xrightarrow{D} \mathcal{N}_C(\mathbf{0}, \boldsymbol{\Gamma}), \tag{21}$$

where $\boldsymbol{\Gamma} = \Xi - \boldsymbol{\Delta}_*\mathcal{F}^{-1}\boldsymbol{\Delta}_*'$.

The model also generates implied marginal probabilities. Consider the 3-item example from above. There are 3 mathematically independent first order marginal probabilities $\dot{\pi}_i$ $(i = 1, 2, 3)$, one per item. There are also 3 mathematically independent second order marginal probabilities $\ddot{\pi}_{ii'}$ for the unique item pairs $(1 \leq i' < i \leq 3)$. In general, these probabilities correspond to the I sets of univariate and $I(I-1)/2$ sets of bivariate margins that can be obtained from the full C-dimensional contingency table using a reduction operator matrix (see e.g., Maydeu-Olivares & Joe, 2006). An example of these marginal probabilities is given by

$$\hat{\boldsymbol{\pi}}_2 = \begin{pmatrix} \dot{\pi}_1 \\ \dot{\pi}_2 \\ \dot{\pi}_3 \\ \ddot{\pi}_{21} \\ \ddot{\pi}_{31} \\ \ddot{\pi}_{32} \end{pmatrix} = \mathbf{L}\hat{\boldsymbol{\pi}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \hat{\pi}_{000} \\ \hat{\pi}_{001} \\ \hat{\pi}_{010} \\ \hat{\pi}_{011} \\ \hat{\pi}_{100} \\ \hat{\pi}_{101} \\ \hat{\pi}_{110} \\ \hat{\pi}_{111} \end{pmatrix}, \tag{22}$$

where $\mathbf{L}$ is an $r \times c$ fixed operator matrix of 0s and 1s that reduces the response pattern probabilities and proportions into marginal probabilities and proportions up to order 2. The $r \times 1$ vector $\hat{\boldsymbol{\pi}}_2 = \mathbf{L}\hat{\boldsymbol{\pi}} = \mathbf{L}\boldsymbol{\pi}(\hat{\boldsymbol{\gamma}}) = \boldsymbol{\pi}_2(\hat{\boldsymbol{\gamma}})$ contains all first and second order model-implied marginal probabilities, evaluated at the maximum likelihood estimate. For dichotomously scored item responses, $r = I + I(I-1)/2$. Obviously $\boldsymbol{p}_2 = \mathbf{L}\boldsymbol{p}$ is the vector of first and second order observed marginal proportions.

A requirement on $\mathbf{L}$ is that it has full row rank, r. This implies that the marginal residual vector $(\boldsymbol{p}_2 - \hat{\boldsymbol{\pi}}_2) = \mathbf{L}(\boldsymbol{p} - \hat{\boldsymbol{\pi}})$ is a full rank linear transformation of the multinomial cell residual vector $(\boldsymbol{p} - \hat{\boldsymbol{\pi}})$. Consequently, the marginal residual vector $(\boldsymbol{p}_2 - \hat{\boldsymbol{\pi}}_2)$ is also asymptotically normal:

$$\sqrt{N}(\boldsymbol{p}_2 - \hat{\boldsymbol{\pi}}_2) = \sqrt{N}\mathbf{L}(\boldsymbol{p} - \hat{\boldsymbol{\pi}}) \xrightarrow{D} \mathcal{N}_r(\mathbf{0}, \boldsymbol{\Gamma}_2), \tag{23}$$

and $\boldsymbol{\Gamma}_2 = \mathbf{L}\boldsymbol{\Gamma}\mathbf{L}' = \mathbf{L}\boldsymbol{\Xi}\mathbf{L}' - \mathbf{L}\boldsymbol{\Delta}_*\mathcal{F}^{-1}\boldsymbol{\Delta}_*'\mathbf{L}' = \boldsymbol{\Xi}_2 - \boldsymbol{\Delta}_{2*}\mathcal{F}^{-1}\boldsymbol{\Delta}_{2*}'$, where $\boldsymbol{\Xi}_2 = \mathbf{L}\boldsymbol{\Xi}\mathbf{L}'$, and $\boldsymbol{\Delta}_{2*} = \mathbf{L}\boldsymbol{\Delta}_*$ is the $r \times d$ Jacobian matrix of the marginal probabilities

$$\boldsymbol{\Delta}_{2*} = \mathbf{L}\frac{\partial \boldsymbol{\pi}(\boldsymbol{\gamma}_*)}{\partial \boldsymbol{\gamma}'} = \frac{\partial \mathbf{L}\boldsymbol{\pi}(\boldsymbol{\gamma}_*)}{\partial \boldsymbol{\gamma}'} = \frac{\partial \boldsymbol{\pi}_2(\boldsymbol{\gamma}_*)}{\partial \boldsymbol{\gamma}'}.$$

Another condition that is important for limited-information model fit testing is that the model must be locally identified from the first and second order marginal probabilities. This local identification is achieved if $\boldsymbol{\Delta}_{2*}$ has full column rank, d.

3.3 The M_2 Test Statistic

The full-information test statistics such as likelihood ratio $G^2$and Pearson's X^2 use residuals based on the full response pattern cross-classifications to test the fit of the model against the general multinomial alternative. The comparison between $\hat{\pi}_{\boldsymbol{y}}$ and $p_{\boldsymbol{y}}$ (on logarithmic or linear scales) leads to well-known goodness of fit statistics such as the likelihood ratio $G^2$and Pearson's X^2:

$$G^2 = 2N\sum_{\boldsymbol{y}} p_{\boldsymbol{y}} \log\frac{p_{\boldsymbol{y}}}{\hat{\pi}_{\boldsymbol{y}}}, X^2 = N\sum_{\boldsymbol{y}} \frac{\left(p_{\boldsymbol{y}} - \hat{\pi}_{\boldsymbol{y}}\right)^2}{\hat{\pi}_{\boldsymbol{y}}}, \tag{24}$$

where the summation is over all C response patterns. Under the null hypothesis that the IRT model fits exactly, these two statistics have the same asymptotic reference distribution, which is a central chi-square with degrees-of-freedom equal to $C - 1 - d$ (Bishop et al., 1975).

Unfortunately as the number of items increases, the number of response patterns increases exponentially. For more than a dozen or so dichotomous items, the contingency table upon which the multinomial is defined becomes sparse for most realistic *N*. It is well known that the asymptotic chi-square approximations for the full-information test statistics break down under sparseness (see e.g., Bartholomew & Tzamourani, 1999).

Recently, limited-information overall fit statistics such as Maydeu-Olivares and Joe's (2006) M_2 have been developed. Limited-information fit statistics use residuals based on lower order (e.g., first and second order) margins of the contingency table. These lower order margins are far better filled when compared to the sparse full contingency table. There is growing awareness that limited-information tests can maintain correct size and can be more powerful than full-information tests (Cai, Maydeu-Olivares, Coffman, & Thissen, 2006; Joe & Maydeu-

Olivares, 2010; Cai & Hansen, 2013). Moreover, Templin (2007) and Jurich, Bradshaw, & DeMars (2014) have demonstrated the potential usefulness of limited-information statistics in evaluating the fit of diagnostic classification models, in particular.

Let $\widehat{\boldsymbol{\Xi}} = diag(\widehat{\boldsymbol{\pi}}) - \widehat{\boldsymbol{\pi}}\widehat{\boldsymbol{\pi}}'$ denote the multinomial covariance matrix evaluated at $\widehat{\boldsymbol{\gamma}}$, and let $\widehat{\boldsymbol{\Xi}}_2 = \mathbf{L}\widehat{\boldsymbol{\Xi}}\mathbf{L}'$. Also evaluate the marginal Jacobian at $\widehat{\boldsymbol{\gamma}}$

$$\widehat{\boldsymbol{\Delta}}_2 = \frac{\partial \boldsymbol{\pi}_2(\widehat{\boldsymbol{\gamma}})}{\partial \boldsymbol{\gamma}'}.$$

When $\widehat{\boldsymbol{\Delta}}_2$ has full column rank, the statistic

$$M_2 = N(\boldsymbol{p}_2 - \widehat{\boldsymbol{\pi}}_2)'\widehat{\boldsymbol{\Omega}}\,(\boldsymbol{p}_2 - \widehat{\boldsymbol{\pi}}_2), \tag{25}$$

where $\widehat{\boldsymbol{\Omega}} = \widehat{\boldsymbol{\Xi}}_2^{-1} - \widehat{\boldsymbol{\Xi}}_2^{-1}\widehat{\boldsymbol{\Delta}}_2\big(\widehat{\boldsymbol{\Delta}}_2'\widehat{\boldsymbol{\Xi}}_2^{-1}\widehat{\boldsymbol{\Delta}}_2\big)^{-1}\widehat{\boldsymbol{\Delta}}_2'\widehat{\boldsymbol{\Xi}}_2^{-1}$, is asymptotically chi-square distributed with $r - d$ degrees-of-freedom under the null hypothesis that the model fits exactly in the population (Browne, 1984). To see that this is the case, we first recognize that from Equation (14), $\sqrt{N}(\boldsymbol{p}_2 - \widehat{\boldsymbol{\pi}}_2)$ is asymptotically a normal random vector with zero means and covariance matrix $\boldsymbol{\Xi}_2 - \boldsymbol{\Delta}_{2*}\mathcal{F}^{-1}\boldsymbol{\Delta}_{2*}'$. By the continuous mapping theorem and the consistency of the maximum likelihood estimator, $\widehat{\boldsymbol{\Omega}}$ converges in probability to the limiting weight matrix $\lim_{N\to\infty}\widehat{\boldsymbol{\Omega}} = \boldsymbol{\Omega}$, where $\boldsymbol{\Omega} = \boldsymbol{\Xi}_2^{-1} - \boldsymbol{\Xi}_2^{-1}\boldsymbol{\Delta}_{2*}(\boldsymbol{\Delta}_{2*}'\boldsymbol{\Xi}_2^{-1}\boldsymbol{\Delta}_{2*})^{-1}\boldsymbol{\Delta}_{2*}'\boldsymbol{\Xi}_2^{-1}$. The product $(\boldsymbol{\Xi}_2 - \boldsymbol{\Delta}_{2*}\mathcal{F}^{-1}\boldsymbol{\Delta}_{2*}')\boldsymbol{\Omega} = \mathbf{I}_r - \boldsymbol{\Xi}_2^{-1}\boldsymbol{\Delta}_{2*}(\boldsymbol{\Delta}_{2*}'\boldsymbol{\Xi}_2^{-1}\boldsymbol{\Delta}_{2*})^{-1}\boldsymbol{\Delta}_{2*}'$ is idempotent and its rank is equal to $r - d$. Therefore, by Cochran's theorem and Slutsky's theorem, M_2 is asymptotically chi-squared with $r - d$ degrees-of-freedom.

When the model does not fit exactly in the population, the quadratic form in M_2 provides a mechanism for computing a Root Mean Square Error of Approximation (RMSEA; Browne & Cudeck, 1993; Maydeu-Olivares, 2013) type index to characterize the degree of model error. This is because the limiting mean of $\sqrt{N}(\boldsymbol{p}_2 - \widehat{\boldsymbol{\pi}}_2)$ will no longer be zero when there does not exist a $\boldsymbol{\gamma}_*$ such that $\boldsymbol{\pi}(\boldsymbol{\gamma}_*) = \boldsymbol{\pi}_*$. Let $\hat{F} = (\boldsymbol{p}_2 - \widehat{\boldsymbol{\pi}}_2)'\widehat{\boldsymbol{\Omega}}\,(\boldsymbol{p}_2 - \widehat{\boldsymbol{\pi}}_2)$ be the observed degree of model error. As per Browne and Cudeck (1993), an unbiased estimate of the population model error is $F_* = \hat{F} - df/N$. The sample RMSEA based on M_2 is defined as a measure of the per degree-of-freedom model error (truncated at 0):

$$\text{RMSEA} = \sqrt{\max\left(\frac{F_*}{df}, 0\right)} \tag{26}$$

Confidence intervals of RMSEA may be easily computed from the noncentral chi-square distribution by following established procedures in Browne and Cudeck (1993).

3.4 Chen and Thissen's (1997) X_{LD}^2 Index

In practice, following a significant overall test, it may be useful to determine the source of the misfit. (This is precisely the motivation in ANOVA, when a significant omnibus F test is followed by pairwise comparisons). Here, we use Chen and Thissen's (1997) X_{LD}^2 index for this purpose, as X_{LD}^2 has proven useful in IRT modeling and, like M_2, is based on marginal residuals. Unlike M_2, for a pair of items, X_{LD}^2 makes use of all proportions and probabilities, not just those that are mathematically independent. For items i and i', the index is defined as

$$X_{LD}^2 = N \sum_{y_i=0}^{1} \sum_{y_{i'}=0}^{1} \frac{\left(p_{y_i y_{i'}} - \hat{\pi}_{y_i y_{i'}}\right)^2}{\hat{\pi}_{y_i y_{i'}}}, \tag{27}$$

where $\hat{\pi}_{y_i y_{i'}}$ is the model-implied bivariate probability for items i and i' in categories y_i and $y_{i'}$, respectively. The analogous bivariate sample proportion is denoted $p_{y_i y_{i'}}$.

With dichotomous data and estimated parameters, X_{LD}^2 is not chi-squared distributed and its limiting mean is less than one (Chen & Thissen, 1997; Liu & Maydeu-Olivares, 2013). However, X_{LD}^2 is often compared to a chi-squared distribution with one degree of freedom, meaning that the index will be conservative under the null hypothesis. Although this may reduce the sensitivity of the index for making judgments of the statistical significance of local dependence for a single item pair, in practice we often use the index to evaluate the relative severity of local independence violations across the many item pairs. Consequently, conservativeness may in fact be a welcome feature under multiplicity of testing.

4 Simulation Studies

In order to evaluate the performance of M_2 and X_{LD}^2 in the context of diagnostic classification modeling, we conducted a series of simulation studies. First, we evaluated the calibration of the test statistics when the fitted model was correctly specified (i.e., matched the generating model; the null condition). We then examined the power of M_2 and X_{LD}^2 to detect a variety of model misspecifications.

For all simulation conditions, the test length was 24 items, and there were four latent attributes. In the data generating Q-matrix, each item loaded onto exactly two of the four attributes. That is, in each row, two elements had a value of zero and two elements had a value of one. Each of the six of the possible rows (i.e., all two-way combinations of the four attributes) appeared four times. The order in which the rows appeared within the Q-matrix was assigned at random.

Rather than sampling slopes and intercepts directly, distributions were instead obtained by specifying distributions of correct response probabilities for respondents that either lack or possess the requisite underlying attributes (i.e., "guessing" and "slipping," respectively). These values were then transformed to match the LCDM parameterization (Henson et al., 2009). The sampling distributions selected for the guessing and slipping parameters were intended to yield values resembling those observed in prior empirical analyses of educational assessment data (see, e.g., de la Torre & Douglas, 2004; Choi et al., 2013; Bradshaw, Izsák, Templin, & Jacobson, 2014). Guessing parameters were drawn from a beta distribution with a mean of 0.25 and standard deviation of 0.05; slipping parameters were drawn from a beta distribution with a mean of 0.15 and standard deviation of 0.05. Item intercepts (α_i) were computed from the guessing parameters (g_i) in the following manner:

$$\alpha_i = -\log\left(\frac{1}{g_i} - 1\right)$$

This intercept, together with the slipping parameter (s_i), was then used to obtain the slope parameter:

$$\gamma_i = -\log\left(\frac{1}{1 - s_i} - 1\right) - \alpha_i$$

In addition to the latent attribute variables, items were also influenced in some data generating conditions by six group-specific dimensions (i.e., testlet effects). The slopes (β) of the items on these dimensions were equal within a data generating condition and assumed a value of 0 (i.e., no testlet effects), 1, or 2. These values were chosen to be typical of testlet effects observed in empirical analyses (e.g., Cai et al., 2011). The Q-matrix and the item parameters used in data generation are presented in Table 1.

Insert Table 1 about here

Various higher-order structures were used to generate the distribution of the latent attributes (the x variables). Models with a single higher-order dimension utilized a one-parameter logistic (1PL) IRT model for the higher-order part, with slope $a = 1.5$ for all attributes and intercepts of $c_1 = -0.45,\ c_2 = 0.15, c_3 = -0.15,\ c_4 = 0.45$. Scores for the higher-order dimension were sampled from either a standard normal density or from one of four non-normal densities illustrated in Figure 1. The non-normal distributions were parameterized as Davidian curves (Woods and Lin, 2009), each with mean 0 and variance 1. The four densities can be described as Bimodal ($\partial_1 = -0.10,\ \partial_2 = 1.98$), Extreme Bimodal ($\partial_1 = -0.52, \partial_2 = 2.29$), Right-skewed ($\partial_1 = 0.69,\ \partial_2 = 4.09$), and Extreme Right-skewed ($\partial_1 = .79,\ \partial_2 = 6.58$), where ∂_1 and ∂_2 are the skewness and kurtosis coefficients, respectively. These densities are similar to those used previously in research on non-normal latent trait density estimation in IRT (see, e.g., Woods & Lin, 2009).

Insert Figure 1 about here

In addition to the univariate normal and non-normal higher-order distributions, we also generated data from a model in which the higher-order structure was multidimensional. For these conditions, attributes 1 and 2 loaded onto one dimension (θ_1), and attributes 3 and 4 loaded onto a second dimension (θ_2). The means of the two higher-order dimensions were 0, their variances were 1, and the correlation between domains varied across conditions ($\rho = 0.4, 0.6, 0.8$).

Figure 2 presents path diagrams for the three basic model structures: a higher-order DINA model (top panel), a DINA model with correlated higher-order dimensions (middle panel), and a higher-order DINA with testlet effects (bottom panel). For each data generating condition, 500 datasets were generated in three sample sizes ($N = 500, 1000, 2000$).

Insert Figure 2 about here

The fitted models used with each data generating condition are summarized in Table 2. The first rows of Table 2 describe the null conditions, and the remaining sections identify the various misspecified models fit within each generating condition. The first category of model misspecification was the failure to account for testlet effects in the fitted model when such effects were part of the data generating models (i.e., when $\beta = 1$ or $\beta = 2$). The second category consisted of misspecifications of the higher-order latent variable distribution. This included fitting models that assume normality in the higher-order dimension when the actual distribution was nonnormal in one of the ways described above and shown in Figure 1 (moderately bimodal, extremely bimodal, or extremely skewed). Also included in this category were conditions in which the attribute distributions were generated from a two-dimensional (rather than one-dimensional) higher-order structure. The final category of misspecification consisted of errors in the characterization of the relationship between items and attributes. This category included specification of the wrong form of the diagnostic model. Specifically, the fitted model specified a compensatory (C-RUM) model for one or all of the test items (rather than DINA, as in the generating model). This category also included four kinds of Q-matrix misspecification: the omission of a path (i.e., changing values of the Q-matrix from 1 to 0), the omission of an attribute variable (i.e., deleting a column of the Q-matrix or), the specification of extraneous paths (i.e., changing values of the Q-matrix from 0 to 1), and the specification of an extraneous attribute (i.e. adding a column to the Q-matrix with some nonzero elements).

The Q-matrix, the form of the item response model, and assumptions about latent variable distributions and overall dimensionality may all contribute to expectations concerning the frequency of particular item response patterns (i.e., model-implied frequencies). For example, if two items are both influenced by a particular attribute (e.g., a high probability of endorsement or correct response requires the attribute) but our model fails to specify that common influence (a kind of Q-matrix error), we may find that the model-implied association between the items is lower than the association observed in the data. Fit statistics based on differences in the observed and expected marginal probabilities (univariate and bivariate, for the test statistics considered here) may be sensitive to this misspecification.

Insert Table 2 about here

All data generation was conducted using the R software (R Development Core Team, 2008). Model estimation and goodness-of-fit computations were conducted with the flexMIRT® item response modeling software (Cai, 2015). An online appendix to this paper includes the flexMIRT® input files used in these simulations, as well as sample data files from the various data generating conditions. Additional guidance on how to specify diagnostic classification models within flexMIRT® and request goodness-of-fit statistics including M_2 and X_{LD}^2 can be found in the flexMIRT® user manual (Houts & Cai, 2015).

4.1 Calibration of the Test Statistic (Type I Error)

Results for M_2 under the null conditions are shown in Table 3. Across the models evaluated—and for each sample size considered—the mean, variance, and empirical rejection rates obtained for the statistic across replications are close to what would be expected. Two-tailed Kolmogorov-Smirnov tests were used to evaluate the extent to which the observed distribution of M_2 differed from the expected chi-square reference distribution. At the $\alpha = 0.05$ level, the Kolmogorov-Smirnov test was not significant under any of the null conditions. The quantile-quantile plots in Figure 3 also show a strong correspondence between the observed and expected distributions of the test statistic.

Insert Table 3 about here

Insert Figure 3 about here

Figure 4 shows a histogram of the empirical rejection rates for the Chen and Thissen (1997) X_{LD}^2 statistic, across the 276 item pairs. These rejection rates were obtained by tallying the number of times X_{LD}^2 exceeded the $\alpha = 0.05$ critical value for a chi-squared distribution with one degree of freedom. The rejection rate is generally below the nominal level, averaging between 0.025 and 0.028 for the null conditions. The fact that X_{LD}^2 is somewhat conservative for

dichotomous data is consistent with results obtained in item response theory modeling (Chen & Thissen, 1997; Liu & Maydeu-Olivares, 2013), as mentioned earlier.

Insert Figure 4 about here

4.2 Power to Detect Unmodeled Testlets

Results presented in Section 4.1 demonstrated that M_2 had very good Type I error control when a hierarchical model was fit to data generated with testlets. Here, we examine results obtained when a standard higher-order diagnostic model—that is, a model that ignores the testlet structure of the data generating model—is fit to the same data. As shown in Table 4, this model was rejected for every replication and at all α levels, regardless of the magnitude of the testlet effect or the sample size. It seems, then, that M_2 is extremely sensitive to this type of model misspecification for the range of conditions we evaluated.

Insert Table 4 about here

Figure 5 provides heat maps depicting the average X_{LD}^2 value (across replications) for each item pair. Darker values indicate larger values of the statistic. The patterns of local dependence revealed through X_{LD}^2 are consistent with the known structure of the generating model. The fitted model does not adequately explain the strong covariation among items within each testlet, resulting in rather severe local dependence among these items.

Insert Figure 5 about here

4.3 Power to Detect Misspecifications of the Higher-order Structure

Results presented in this section were obtained by fitting a standard higher-order DINA model (i.e., one in which the higher-order dimension is univariate normal) to data generated from models with non-standard higher-order structures. The data generating models included

higher-order latent dimension distributions that were non-normal or bivariate normal. Table 5 presents the M_2 empirical rejection rates for these conditions of model misspecification.

Insert Table 5 about here

Empirical rejection rates for the non-normal generating conditions are quite similar to the nominal α levels, indicating that M_2 is not sensitive to this type of misspecification. This result is consistent with a previous study examining the power of M_2 to detect non-normality in item response theory models (Li & Cai, 2012).

The results for the data generated from models with two higher-order dimensions varied according to the correlation between these dimensions. Specifically, rejection rates increased as the correlation decreased (that is, as the higher-order structure of the generating model became less similar to the undimensional structure of the fitted model). When the correlation was $\rho = 0.8$, the rejection rates were only slightly elevated above the nominal α levels. Power was higher when $\rho = 0.4$, though still fairly low except for the largest sample size examined.

4.4 Power to Detect Misspecifications of the Q-matrix or the Item Model Type

Table 6 presents results for conditions in which there were errors in the Q-matrix of the fitted model or misspecification of the item model type. As described earlier, the Q-matrix errors included the addition or omission of paths (i.e., changing the values of individual Q-matrix elements, from 0 to 1 or vice versa) and the addition or omission of latent attributes (i.e., adding or deleting a column from the Q-matrix). For errors of model type, a compensatory (C-RUM) model was specified for either one item or for all items (the data were generated according to a DINA model for all items).

Insert Table 6 about here

The M_2 statistic was sensitive to three of the four kinds of Q-matrix missspecification examined. There was good power to detect the addition or omission of paths. Rejection rates

were higher than the nominal α levels when a latent attribute was omitted. However, power to detect this error was good only for the highest sample size examined (when $N = 2000$ and $\alpha = 0.05$, the rejection rate was 0.888). In contrast, specification of extraneous attribute appeared to have no effect on the rejection rates, which were similar to the nominal α levels. Figure 6 shows the patterns of local dependence for these conditions, as reflected in the average X^2_{LD} values. The X^2_{LD} statistic clearly identified items with incorrect Q-matrix misspecifications, so long as the number of such misspecifications was small (the pattern of local dependence resulting from the omission of an attribute—which affects a much larger number of variables—would seem to be less interpretable).

Insert Figure 6 about here

When an extraneous attribute is included in the model, neither M_2 nor X^2_{LD} provide evidence of misspecification. However, inspection of the marginal attribute probabilities reveals that the expected probability of possessing the extraneous attribute is very close to 1. In a DINA model, then, it seems that such a variable can be absorbed without any change in model fit. In the example here, the extraneous attribute (x_5) nearly always takes a value of 1. In those cases, the third-order interaction is the same as the corresponding second order interaction (that is, if $x_5 = 1$, then $x_j x_{j'} x_5 = x_j x_{j'}$). As a result, the parameters estimated end up representing the same quantity ($\hat{\lambda}_{j \times j' \times 5} \approx \hat{\lambda}_{j \times j'}$).

The M_2 statistic appears to have some sensitivity to the misspecification of item type. However, when the error is limited to a single item, rejection rates are only slightly above the nominal rates. Power is substantially higher when this misspecification is applied to all items in the test. For the conditions examined, X^2_{LD} does not appear to be particularly informative, as shown in Figure 7.

Insert Figure 7 about here

5 Analysis of Empirical Data

The results of the simulation study presented in Section 4 suggest that fit statistics based on univariate and bivariate marginal subtables can be useful in identifying and characterizing certain kinds of model misfit. Here, we apply the proposed approach to an empirical example, using M_2 and the Chen and Thissen (1997) X^2_{LD} statistic to evaluate the fit of alternative diagnostic models to data from the 2007 Trends in Mathematics and Science Study (TIMSS). This example builds on prior work by Lee, Park, & Taylan (2011), who analyzed data from booklets 4 and 5 from the TIMSS 2007 fourth grade mathematics test. As part of their study, several teachers and content experts reviewed and coded the TIMSS test items according to the specific testing objectives described in the TIMSS 2007 framework. For the 25 items considered in the study, 15 unique testing objectives were identified (out of the 32 objectives in the test framework). Accordingly, the Q-matrix proposed by Lee et al. (2011)—shown in their Table 3—consists of 25 rows (one for each item) and 15 columns (with each attribute representing the skill or ability implicit in one testing objective).

There is a good deal of variation in the number of items measuring each attribute. Ten of the 15 attributes are measured by only two or three items, while the second and third attributes are measured by 16 and 11 items, respectively. Among the 25 items, the number of underlying attributes ranges from 1 (items 2, 9, 24) to 6 (item 14).

Lee et al. (2011) specified a conjunctive (DINA) model for the items in their analysis. For the current study, we initially fit a higher-order version of this model (de la Torre & Douglas, 2004) using the Q-matrix exactly as reported in the earlier study to a sample of 564 students from the United States. As shown in the first row of Table 7, the value of M_2 for this model (model 1) was 391.0, with 259 degrees of freedom. The RMSEA based on M_2 has a value of 0.030, with 90% confidence interval of (0.000, 0.036).

Insert Table 7 about here

Values of the Chen and Thissen (1997) X^2_{LD} statistic are presented for this model (model 1) in the left panel of Figure 8. There are a handful of item pairs with fairly large X^2_{LD} values,

indicating substantial local dependence. For illustrative purposes, we focused our attention here on the two item pairs with the largest X^2_{LD} values: items 1—5 ($X^2_{LD} = 13.8$), and items 18—19 ($X^2_{LD} = 38.0$). Table 8 presents the observed marginal response proportions and model-implied probabilities from which the test statistic was computed.

Insert Figure 8 about here

Insert Table 8 about here

We examined the two item pairs and their specification within the initial fitted model for potential causes of the observed local dependence. The items considered in this study have all been released (Foy & Olson, 2009) and were thus available for review. Items 18 and 19 are administered within a cluster or testlet (M031242A/B/C), and it was evident upon inspecting the items that a correct response to item 18 (M031242A) would seem to greatly simplify the task of answering item 19. Specifically, the answer to item 19 (M031242C) can quite simply be read from a table that the examinee is asked to complete for item 18. This may explain why the initial model does not fully explain the covariation in responses between these two items. Although it would be possible to arrive at the correct answer to item 19 by applying the skills identified in the Q-matrix as being relevant, those skills are less necessary once an examinee answers item 18. In order to model this dependence between these items (conditional on the attributes), a testlet effect could be specified. It should be noted that item 20 (M031242C) is also part of the same item cluster. However, this item does not rely quite as directly on information from items 18 or 19, so we chose to ignore local dependence between item 20 and items 18 and 19. Items 9 and 10 (M041258A and M041258B, respectively) also comprise a testlet but show very little evidence of local dependence, so no random effect is specified for this pair.

Our review of items 1 and 5 identified two possible changes in the Q-matrix. First, although item 1 (M041052) had been described in the study by Lee et al. (2011) as requiring both attributes 1 and 2, it seemed to us that possession of attribute 1 would be sufficient to obtain the correct answer. Thus, we posited an alternative Q-matrix specification for item 1, with this item

depending only on possession of attribute 1. After examination of item 5, we concluded that the specification of dependence on attributes 2 and 3 was reasonable. However, the relevance of attribute 8 was unclear. Thus, a second Q-matrix change was considered, with item 5 depending on attributes 2 and 3 but not attribute 8.

In sum, our alternative model for the TIMSS data included three changes. Two changes were made to the Q-matrix: the values of elements $q_{1,2}$ and $q_{5,8}$ were changed from 1 to 0. In addition, a testlet effect was added to account for the strong dependence between items 18 and 19. The total number of estimated parameters is 67 for the alternative model—one more than required for the initial model. The Q-matrix changes for items 1 and 5 do not affect the number of free parameters. For item 1, the interaction $\gamma_{1,1\times2}$ is fixed to 0, but the main effect $\gamma_{1,1}$ is now estimated. Similarly, for item 5, the third-order interaction $\gamma_{5,2\times3\times8}$ is fixed to 0, and $\gamma_{5,2\times3}$ is estimated. The one additional parameter estimated in the alternative model is the slope parameter for the testlet effect (for identification, the slopes of items 18 and 19 were constrained to be equal—i.e., $\beta_{18,1} = \beta_{19,1} = \beta$).

Overall goodness-of-fit indices for the alternative model (model 2) are presented in the second row of Table 7. The value of M_2 for the alternative model was 330.3, with 258 degrees of freedom. The RMSEA based on M_2 has a value of 0.022, with 90% confidence interval of (0.000, 0.029). Results for the Chen & Thissen (1997) X_{LD}^2 are shown in the second row of Table 8 and in the right panel of Figure 8. In summary, the fit of the alternative model is slightly improved over the initial model, both on the basis of the limited-information fit statistics (including the RMSEA values derived from M_2) and the information-based indices (AIC and BIC). It should be noted, however, that this improvement is rather modest. In addition, while specification of the testlet effect seems to have fully accounted for the local dependence of items 18 and 19 (with X_{LD}^2 decreased from 38.0 to 0.9), there remains some dependence between items 1 and 5 (X_{LD}^2 only decreased from 13.8 to 11.0), despite the changes in model specification.

Of course, for this empirical study, we cannot know the true generating model. That said, our analyses are primarily intended to illustrate the ways in which researchers might use goodness-of-fit statistics to evaluate the fit of models, to characterize possible misspecifications, and to identify candidate alternative models (and then test these alternatives, though ideally

this would be done with an independent cross-validation sample of respondents to avoid capitalizing on chance).

6 Discussion

In this paper, we demonstrate the application of limited-information fit statistics to diagnostic classification models. In doing so, we address a well-known gap in the practice of diagnostic modeling (e.g., Maris & Bechger, 2009; Wilhelm & Robitzsch, 2009; Rupp et al., 2010). Through simulation studies we found that M_2 is well-calibrated, closely matching its reference distribution. This result was observed across a wide range of conditions, including standard higher-order diagnostic classification models, hierarchical models (e.g., with testlet effects), and models with correlated higher-order dimensions.

We also examined the sensitivity of M_2 to a number of different kinds of model misspecification, including (1) failure to account for testlet-type effects (i.e., unmodeled dimensions), (2) incorrect specification of higher-order distribution or structure (fitting higher-order models with univariate normal distributions of the higher-order dimension to data generated from non-normal or bivariate normal distributions, (3) errors in the Q-matrix, and (4) misspecifications of item type (C-RUM instead of DINA). The results here were mixed. M_2 was found to be highly sensitive to the presence of testlet effects and certain Q-matrix misspecifications (addition or omission of paths; the omission of a latent attribute was also detectable, but power was rather low except at the highest sample size examined). In contrast, M_2 was largely insensitive to misspecifications of the higher-order structure. Misfit was not detected when the higher-order dimension was sampled from any of the non-normal distributions examined. When the generating model included correlated higher-order dimensions, power was relatively low for strongly correlated dimensions but increased as the correlation decreased.

As a complement to the test of overall fit, we examined the usefulness of Chen and Thissen's (1997) local dependence statistic X^2_{LD}. While M_2 is computed from all the univariate and bivariate subtables, X^2_{LD} is computed from the bivariate subtable for a single item pair. In that sense, X^2_{LD} may be viewed as a *post hoc* test for multiple comparisons, allowing for possible

sources of overall model misfit to be identified. Indeed, we observed that certain kinds of model misspecification produce signatures of local dependence. These patterns of dependence may implicate particular items and item pairs (or larger clusters). In such cases, items might be scrutinized for evidence of Q-matrix errors, unmodeled dependencies across items, or misspecifications in the type of diagnostic model being applied.

There are, of course, many limitations to the work presented here. First, we have focused on the application of M_2 to dichotomous item response data. It would be useful, however, to examine the performance of the test statistic with polytomous models. Prior work has suggested that even bivariate marginal subtables may be poorly filled as the number of categories increases, potentially reducing the utility of M_2 (Cai & Hansen, 2013). Various methods for collapsing the subtables have been proposed and seem to perform well in applications of item response theory (Joe & Maydeu-Olivares, 2010; Maydeu-Olivares, Cai, & Hernandez, 2011; Cai & Hansen, 2013; Cai & Monroe, 2014); these approaches should be evaluated in the context of diagnostic classification modeling.

A second limitation is that in our simulation study we held constant certain aspects of the data generating model. For example, the number of attributes ($K = 4$), the number of test items ($I = 24$), the structure of the Q-matrix, and the item type (DINA) were the same across all conditions. Although this was done in order to put some bounds on the scope of this study, one might reasonably wonder whether some of our findings might differ if any of these features were allowed to vary. It is noteworthy, then, that the test statistics utilized here—M_2 and the Chen and Thissen (1997) X^2_{LD}—have been implemented for diagnostic classifications models in the flexMIRT® item response modeling software (Cai, 2015). We expect that increased availability of these tools for evaluating fit will further clarify their potential utility, as well as their limitations.

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Table 1. Data generation for simulation study: Q-matrix and item parameters.

i	Q-matrix				α_i	attribute two-way interaction terms						testlet slope parameters					
	$q_{i,1}$	$q_{i,2}$	$q_{i,3}$	$q_{i,4}$		$\gamma_{i,1x2}$	$\gamma_{i,1x3}$	$\gamma_{i,1x4}$	$\gamma_{i,2x3}$	$\gamma_{i,2x4}$	$\gamma_{i,3x4}$	$\beta_{i,1}$	$\beta_{i,2}$	$\beta_{i,3}$	$\beta_{i,4}$	$\beta_{i,5}$	$\beta_{i,6}$
1	0	1	1	0	-1.29	.00	.00	.00	3.76	.00	.00	(0,1,2)	.00	.00	.00	.00	.00
2	1	1	0	0	-1.04	3.00	.00	.00	.00	.00	.00	(0,1,2)	.00	.00	.00	.00	.00
3	0	1	1	0	-1.36	.00	.00	.00	2.90	.00	.00	(0,1,2)	.00	.00	.00	.00	.00
4	1	0	1	0	-1.00	.00	2.06	.00	.00	.00	.00	(0,1,2)	.00	.00	.00	.00	.00
5	1	0	1	0	-1.36	.00	3.14	.00	.00	.00	.00	.00	(0,1,2)	.00	.00	.00	.00
6	0	1	0	1	-.95	.00	.00	.00	.00	2.51	.00	.00	(0,1,2)	.00	.00	.00	.00
7	0	0	1	1	-.87	.00	.00	.00	.00	.00	2.63	.00	(0,1,2)	.00	.00	.00	.00
8	0	0	1	1	-1.19	.00	.00	.00	.00	.00	3.61	.00	(0,1,2)	.00	.00	.00	.00
9	0	1	1	0	-.59	.00	.00	.00	2.52	.00	.00	.00	.00	(0,1,2)	.00	.00	.00
10	0	1	0	1	-.98	.00	.00	.00	.00	2.90	.00	.00	.00	(0,1,2)	.00	.00	.00
11	0	1	0	1	-1.29	.00	.00	.00	.00	3.05	.00	.00	.00	(0,1,2)	.00	.00	.00
12	0	1	0	1	-.74	.00	.00	.00	.00	1.94	.00	.00	.00	(0,1,2)	.00	.00	.00
13	1	0	1	0	-1.11	.00	2.92	.00	.00	.00	.00	.00	.00	.00	(0,1,2)	.00	.00
14	1	0	0	1	-1.10	.00	.00	2.95	.00	.00	.00	.00	.00	.00	(0,1,2)	.00	.00
15	1	1	0	0	-.80	2.21	.00	.00	.00	.00	.00	.00	.00	.00	(0,1,2)	.00	.00
16	1	0	0	1	-.84	.00	.00	2.32	.00	.00	.00	.00	.00	.00	(0,1,2)	.00	.00
17	1	0	0	1	-.92	.00	.00	2.97	.00	.00	.00	.00	.00	.00	.00	(0,1,2)	.00
18	1	0	0	1	-.81	.00	.00	2.87	.00	.00	.00	.00	.00	.00	.00	(0,1,2)	.00
19	1	0	1	0	-.85	.00	2.42	.00	.00	.00	.00	.00	.00	.00	.00	(0,1,2)	.00
20	1	1	0	0	-1.08	2.45	.00	.00	.00	.00	.00	.00	.00	.00	.00	(0,1,2)	.00
21	0	0	1	1	-1.81	.00	.00	.00	.00	.00	3.60	.00	.00	.00	.00	.00	(0,1,2)
22	1	1	0	0	-.91	2.23	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	(0,1,2)
23	0	0	1	1	-1.12	.00	.00	.00	.00	.00	2.67	.00	.00	.00	.00	.00	(0,1,2)
24	0	1	1	0	-1.15	.00	.00	.00	3.17	.00	.00	.00	.00	.00	.00	.00	(0,1,2)

Note: In generating model (DINA), the attribute main effects (which are not shown) are fixed to zero.

Table 2. Summary of data generating and fitted models used in simulation study.

data generating model			fitted model		
higher-order structure	attribute model	testlets	higher-order structure	attribute model	testlet
null (correctly specified) models (results in Table 3)					
univariate normal	DINA	no	univariate normal	DINA	no
univariate normal	DINA	yes ($\beta = 1$)	univariate normal	DINA	yes
univariate normal	DINA	yes ($\beta = 2$)	univariate normal	DINA	yes
bivariate normal ($\rho = 0.4$)	DINA	no	bivariate normal	DINA	no
bivariate normal ($\rho = 0.6$)	DINA	no	bivariate normal	DINA	no
bivariate normal ($\rho = 0.8$)	DINA	no	bivariate normal	DINA	no
failure to model testlet effects (results in Table 4)					
univariate normal	DINA	yes ($\beta = 1$)	univariate normal	DINA	no
univariate normal	DINA	yes ($\beta = 2$)	univariate normal	DINA	no
misspecifications of higher-order latent variable distributions (results in Table 5)					
univariate bimodal	DINA	no	univariate normal	DINA	no
univariate extreme bimodal	DINA	no	univariate normal	DINA	no
univariate right-skewed	DINA	no	univariate normal	DINA	no
univariate extreme right skewed	DINA	no	univariate normal	DINA	no
bivariate normal ($\rho = 0.4$)	DINA	no	univariate normal	DINA	no
bivariate normal ($\rho = 0.6$)	DINA	no	univariate normal	DINA	no
bivariate normal ($\rho = 0.8$)	DINA	no	univariate normal	DINA	no
Q-matrix or item type misspecifications (results in Table 6)					
univariate normal	DINA	no	univariate normal	C-RUM (item 8)	no
univariate normal	DINA	no	univariate normal	C-RUM (all items)	no
univariate normal	DINA	no	univariate normal	omit path	no
univariate normal	DINA	no	univariate normal	add path	no
univariate normal	DINA	no	univariate normal	omit attribute	no
univariate normal	DINA	no	univariate normal	add attribute	no

Table 3. Simulation study results: M_2 calibration under null conditions for various data generating models.

N	reps	df	M	V	KS	empirical rejection rate				
						.200	.150	.100	.050	.010
higher-order DINA										
500	500	247	248.4	518.4	.356	.206	.162	.136	.064	.014
1000	500	247	248.0	508.7	.757	.212	.154	.104	.060	.018
2000	500	247	247.0	524.3	.692	.212	.146	.108	.054	.014
higher-order DINA with testlet effects (testlet slope β=1)										
500	500	241	240.7	450.9	.931	.200	.140	.078	.040	.002
1000	500	241	240.0	436.5	.787	.186	.128	.076	.036	.006
2000	500	241	240.4	499.5	.198	.198	.156	.116	.050	.004
higher-order DINA with testlet effects (testlet slope β=2)										
500	499	241	242.2	459.7	.311	.212	.166	.120	.062	.014
1000	500	241	242.6	450.0	.049	.204	.142	.086	.056	.008
2000	500	241	240.3	435.2	.352	.186	.134	.090	.042	.004
DINA with bivariate normal higher-order latent distribution, ρ=0.4										
500	496	245	245.0	480.8	.913	.179	.139	.101	.050	.008
1000	499	245	246.3	503.0	.146	.220	.160	.106	.062	.010
2000	500	245	243.3	488.5	.079	.186	.140	.078	.040	.016
DINA with bivariate normal higher-order latent distribution, ρ=0.6										
500	483	245	245.5	486.6	.551	.199	.147	.099	.050	.012
1000	498	245	246.6	494.8	.057	.219	.173	.100	.056	.008
2000	500	245	244.0	480.6	.557	.172	.122	.088	.046	.012
DINA with bivariate normal higher-order latent distribution, ρ=0.8										
500	394	245	244.2	473.6	.953	.198	.140	.091	.038	.003
1000	464	245	244.2	480.4	.805	.196	.157	.093	.039	.002
2000	492	245	244.1	481.9	.390	.195	.146	.093	.051	.008

Note: N is the sample size; *reps* is the number of converged replications (out of 500); *df* is the degrees of freedom for M_2, given the fitted model; M and V observed the mean and variance, respectively, of M_2 across the converged replications within the condition; KS indicates the p-values for two-tailed Kolmogorov-Smirnov test.

Table 4. Simulation study results: M_2 power to detect testlet effects.

N	reps	df	empirical rejection rate					RMSEA	
			.200	.150	.100	.050	.010	M	(90% CI)
higher-order DINA with testlet effects (testlet slope β=1)									
500	500	247	1.000	1.000	1.000	1.000	1.000	.044	(.036,.051)
1000	500	247	1.000	1.000	1.000	1.000	1.000	.044	(.040,.048)
2000	500	247	1.000	1.000	1.000	1.000	1.000	.044	(.041,.047)
higher-order DINA with testlet effects (testlet slope β=2)									
500	500	247	1.000	1.000	1.000	1.000	1.000	.114	(.107,.120)
1000	500	247	1.000	1.000	1.000	1.000	1.000	.115	(.110,.120)
2000	500	247	1.000	1.000	1.000	1.000	1.000	.115	(.111,.118)

Note: N is the sample size; reps is the number of converged replications (out of 500); df is the degrees of freedom for M_2, given the fitted model.

Table 5. Simulation study results: M_2 power to detect misspecifications of higher-order latent variable distributions.

N	reps	*df*	empirical rejection rate					RMSEA	
			.200	.150	.100	.050	.010	*M*	(90% CI)
DINA with bimodal higher-order latent variable distribution									
500	500	247	.184	.134	.090	.044	.006	.006	(.000,.017)
1000	500	247	.180	.130	.090	.038	.006	.004	(.000,.012)
2000	500	247	.216	.168	.100	.056	.010	.003	(.000,.009)
DINA with extreme bimodal higher-order latent variable distribution									
500	500	247	.220	.156	.096	.058	.012	.006	(.000,.018)
1000	500	247	.206	.160	.120	.048	.014	.004	(.000,.012)
2000	500	247	.220	.176	.116	.052	.008	.003	(.000,.009)
DINA with right-skewed higher-order latent variable distribution									
500	500	247	.188	.128	.086	.028	.006	.005	(.000,.017)
1000	500	247	.204	.164	.108	.050	.018	.004	(.000,.012)
2000	500	247	.216	.160	.110	.038	.008	.003	(.000,.009)
DINA with extreme right-skewed higher-order latent variable distribution									
500	500	247	.196	.142	.102	.060	.010	.006	(.000,.018)
1000	500	247	.242	.176	.124	.062	.008	.004	(.000,.013)
2000	500	247	.190	.130	.086	.040	.004	.002	(.000,.008)
DINA with bivariate normal higher-order latent distribution, ρ=0.4									
500	500	247	.290	.224	.158	.088	.022	.007	(.000,.019)
1000	500	247	.452	.364	.290	.164	.056	.007	(.000,.015)
2000	500	247	.626	.536	.450	.312	.134	.007	(.000,.012)
DINA with bivariate normal higher-order latent distribution, ρ=0.6									
500	500	247	.246	.190	.124	.064	.022	.006	(.000,.018)
1000	500	247	.330	.252	.174	.092	.026	.006	(.000,.014)
2000	500	247	.416	.332	.246	.150	.036	.005	(.000,.010)
DINA with bivariate normal higher-order latent distribution, ρ=0.8									
500	500	247	.236	.170	.100	.050	.014	.006	(.000,.017)
1000	500	247	.240	.192	.114	.056	.004	.004	(.000,.012)
2000	500	247	.238	.184	.130	.066	.014	.003	(.000,.009)

Note: *N* is the sample size; reps is the number of converged replications (out of 500); *df* is the degrees of freedom for M_2, given the fitted model.

Table 6. Simulation study results: M_2 power to detect to Q-matrix or item type misspecifications.

N	reps	df	empirical rejection rate					RMSEA	
			.200	.150	.100	.050	.010	M	(90% CI)
omit paths from attribute to items ($x_1 \rightarrow y_5$, $x_1 \rightarrow y_{16}$)									
500	500	247	.978	.968	.940	.888	.730	.024	(.015,.032)
1000	500	247	1.000	1.000	1.000	1.000	.998	.024	(.019,.029)
2000	500	247	1.000	1.000	1.000	1.000	1.000	.025	(.021,.028)
add (extraneous) paths from *attribute to items ($x_1 \rightarrow y_3$, $x_1 \rightarrow y_{23}$)*									
500	500	247	.920	.892	.850	.772	.566	.021	(.010,.029)
1000	500	247	1.000	1.000	1.000	1.000	.984	.022	(.017,.027)
2000	500	247	1.000	1.000	1.000	1.000	1.000	.022	(.019,.025)
omit attribute (x_4)									
500	500	248	.472	.392	.306	.206	.064	.010	(.000,.021)
1000	500	248	.738	.680	.590	.452	.202	.011	(.000,.019)
2000	500	248	.974	.956	.940	.888	.740	.012	(.007,.016)
add (extraneous) attribute (x_5)									
500	500	246	.204	.166	.138	.058	.012	.006	(.000,.018)
1000	500	246	.206	.154	.108	.056	.018	.004	(.000,.012)
2000	499	246	.206	.148	.100	.054	.012	.003	(.000,.009)
apply an incorrect item type (C-RUM for item 8)									
500	500	246	.230	.180	.138	.066	.018	.006	(.000,.018)
1000	500	246	.246	.186	.128	.074	.018	.004	(.000,.013)
2000	500	246	.280	.208	.144	.076	.024	.003	(.000,.009)
apply an incorrect item type (C-RUM for all items)									
500	500	223	.966	.952	.932	.866	.710	.025	(.014,.034)
1000	500	223	1.000	1.000	1.000	1.000	.990	.025	(.020,.031)
2000	500	223	1.000	1.000	1.000	1.000	1.000	.026	(.022,.029)

Note: N is the sample size; reps is the number of converged replications (out of 500); df is the degrees of freedom for M_2, given the fitted model.

Table 7. Empirical illustration: Overall goodness-of-fit evaluation for the two fitted models.

	df	M_2	p	RMSEA	(90% C.I.)	AIC	BIC
model 1	259	391.0	<.001	.030	(.000, .036)	15872.4	16158.5
model 2	258	330.3	.002	.022	(.000, .029)	15821.3	16111.8

Note: Model 1 is a higher-order DINA model with Q-matrix as described by Lee, Park, & Taylan (2011). The alternative model (model 2) has a slightly altered Q-matrix and adds a testlet effect (for items 18—19).

Table 8. Empirical illustration: Bivariate marginal response pattern observed proportions and model-implied probabilities for 2 item pairs (1—5 and 18—19) and corresponding X^2_{LD} values for the two fitted models.

	observed				model-implied				X^2_{LD}	p
	p_{00}	p_{01}	p_{10}	p_{11}	$\hat{\pi}_{00}$	$\hat{\pi}_{01}$	$\hat{\pi}_{10}$	$\hat{\pi}_{11}$		
items 1,5										
model 1	.128	.073	.220	.580	.097	.103	.252	.549	13.8	< .001
model 2					.103	.101	.250	.546	11.0	< .001
items 18,29										
model 1	.314	.046	.232	.408	.257	.104	.291	.348	38.0	< .001
model 2					.310	.053	.241	.396	0.9	.331

Note: Model 1 is a higher-order DINA model with Q-matrix as described by Lee, Park, & Taylan (2011). The alternative model (model 2) has a slightly altered Q-matrix and adds a testlet effect (for items 18—19).

Figure Captions

Figure 1. *Densities from which scores on the higher-order dimension were sampled for non-normal data generating conditions.*

Figure 2. *Path diagrams for data generating models used in simulation study. Test items are indicated by boxes. The horizontal lines through these boxes represent thresholds and indicate that the items are dichotomous, rather than continuous. The latent variables are indicated by open circles. Attribute variables have horizontal lines passing through the circles. These again represent thresholds and indicate that these variables (like the test items) are dichotomous (the higher-order dimensions and testlet effects, in contrast, are continuous). Directional arrows indicate loadings of the items onto the latent variables and loadings of the latent attributes onto higher-order variables. Following the notation of Rupp et al. (2010, p. 47; see also Bradshaw et al., 2014, p. 8), attribute interactions are indicated by the small closed circles (where paths from attributes to items converge). The bidirectional arrow (in panel B) indicates the correlation between higher-order dimensions.*

Figure 3. *Simulation study results: Quantile–quantile plots of observed* M_2 *values and their reference chi-square distributions (degrees of freedom shown in the subscripts of the x-axis labels). Closed grey circles indicate results for conditions with sample size N = 500, open black circles indicate results for N = 1000, and plus signs indicate N=2000. Reported p-values are for a two-tailed Kolmogorov–Smirnov test of the equality of the observed* M_2 *distributions with its corresponding reference distribution.*

Figure 4. *Simulation study results: Empirical rejection rates for Chen and Thissen (1997)* X^2_{LD} *across all item pairs. Results are shown for null conditions (fitted model correctly specified) with sample size N=2000 and* α*=0.05. Rejection rates are based on all converged replications (minimum of 492; maximum of 500).*

Figure 5. *Simulation study results: Chen and Thissen (1997)* X^2_{LD} *heat map for diagnostic models with testlet effects. Shading is based on the average RMSEA for the item pair across all converged replications. The generating model in both panels is a higher-order DINA model with testlet*

effects. The testlet slope parameters are β=1 and β=2 for the left and right panels, respectively. The fitted models do not include the testlet effects.

Figure 6. *Simulation study results: Chen and Thissen (1997) X^2_{LD} heat map for diagnostic models with incorrect specification of item type. Shading is based on the average RMSEA for the item pair across all converged replications. The generating model is a higher-order DINA model. In the left panel, item 8 (indicated by tick mark on the x- and y-axes) is incorrectly specified as C-RUM. In the right panel, all 24 items are incorrectly specified as C-RUM.*

Figure 7. *Simulation study results: Chen and Thissen (1997) X^2_{LD} heat map for diagnostic models with Q-matrix misspecification. Shading is based on the average RMSEA for the item pair across all converged replications. The generating model in all four panels is a higher-order DINA model. In top-left panel, paths from x_1 to y_5 and from x_1 to y_{16} are omitted (i.e., the values of Q-matrix elements $q_{5,1}$ and $q_{16,1}$ were changed from 1 to 0; tickmarks identify items 5 and 16). In the top-right panel, extraneous paths were created from x_1 to y_3 and from x_1 to y_{23} (i.e., the values of Q-matrix elements $q_{3,1}$ and $q_{23,1}$ were changed from 0 to 1; tickmarks identify items 3 and 23). In the bottom-left panel, attribute x_4 is omitted (i.e., all values in column 4 of the Q-matrix are 0; 12 elements that have values of 1 in the Q-matrix of the generating model are identified by tickmarks). In the bottom-right panel, an extraneous attribute, x_5 is specified (i.e., a 5th column is added to the Q-matrix); 4 items (2,6,8, and 13); indicated by tickmarks on the x- and y-axes) have Q-matrix values of 1 for this attribute.*

Figure 8. *Results from empirical illustration: Chen and Thissen (1997) X^2_{LD} heat map for analysis of 25 items from TIMSS 4th grade math booklet 4. Left panel (model 1) shows results obtained by fitting a higher-order DINA model with Q-matrix as described by Lee, Park, & Taylan (2011). Right panel (model 2) shows results obtained by fitting a model with a slightly altered Q-matrix and the addition of a testlet effect (for items 18—19).*

Figure 1

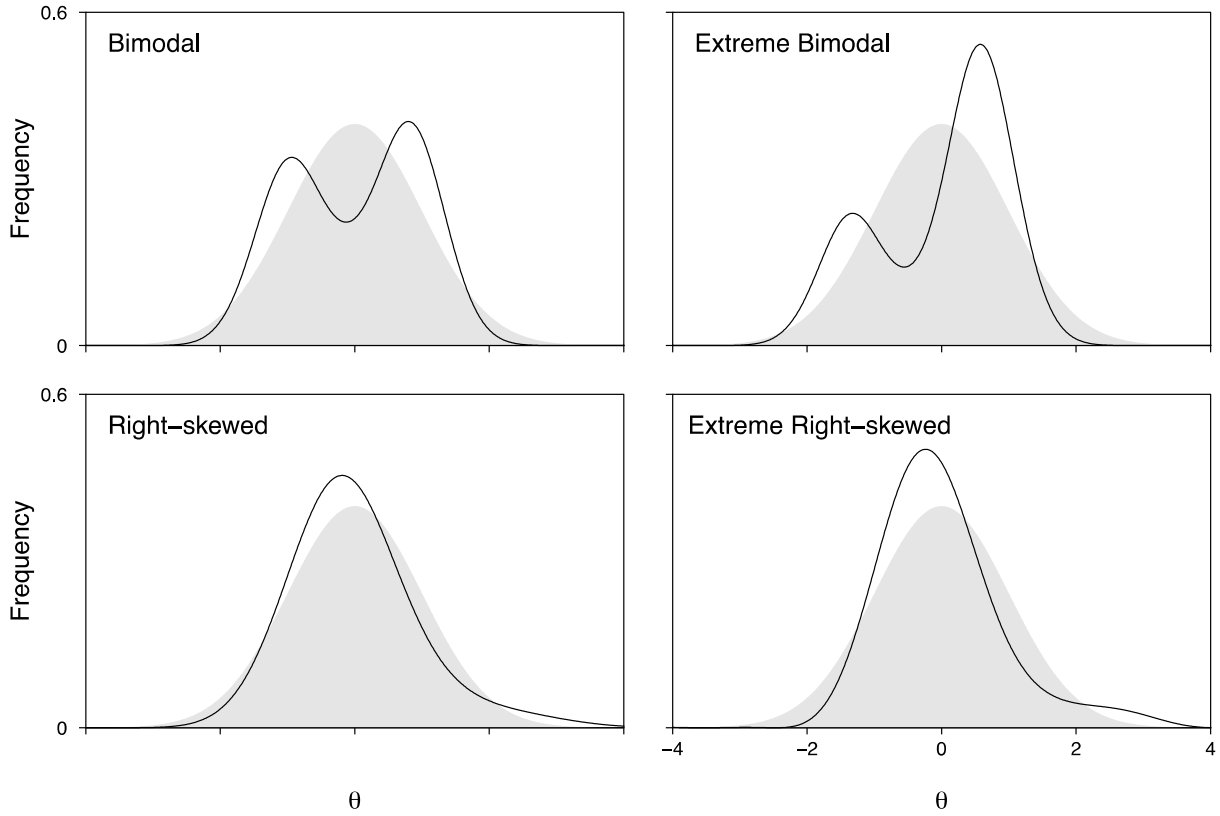
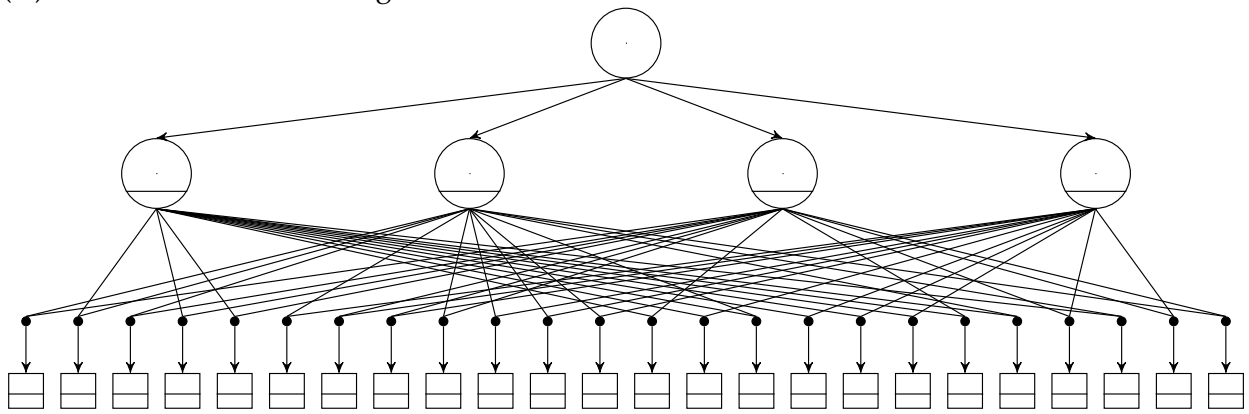
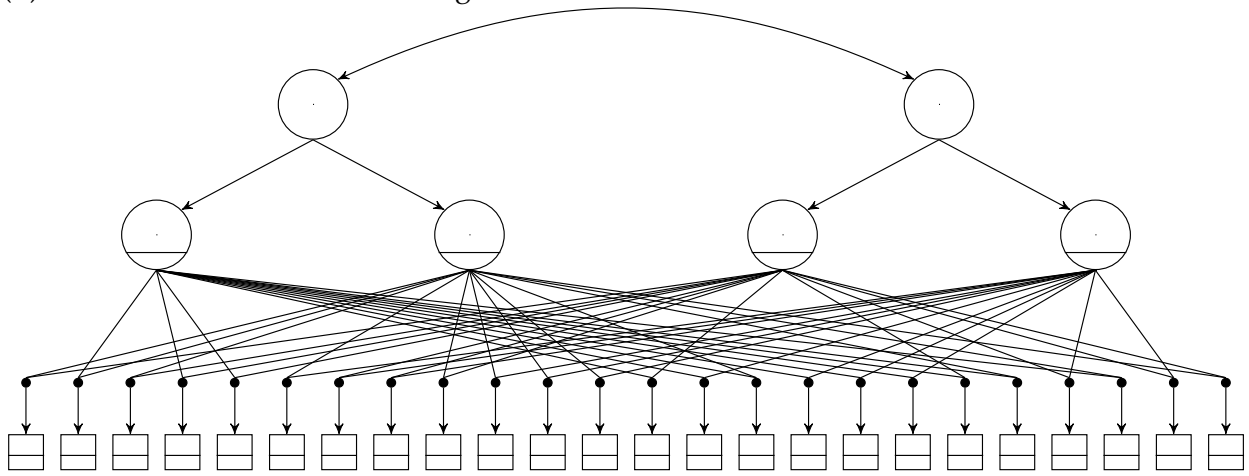

Bimodal
Extreme Bimodal
Right−skewed
Extreme Right−skewed
Frequency
Frequency
0.6
0
0.6
0
−4
−2
0
2
4
θ
θ

Figure 2

(A) DINA model with one higher-order dimension



(B) DINA model with correlated higher-order dimensions



(C) DINA model with one higher-order dimension and six testlets

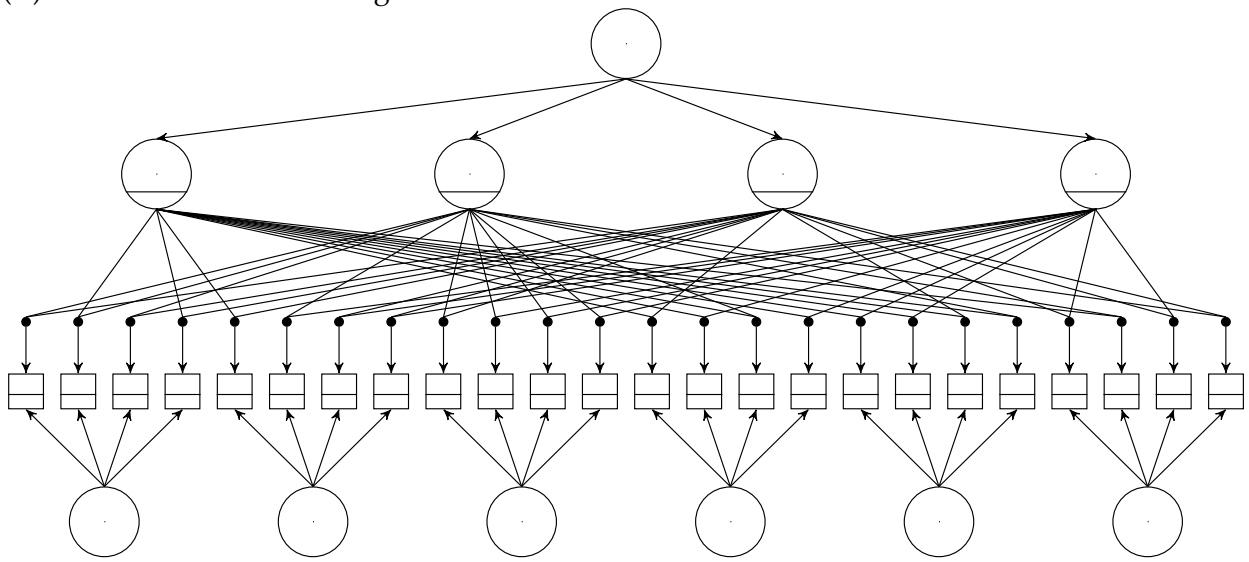


Figure 3

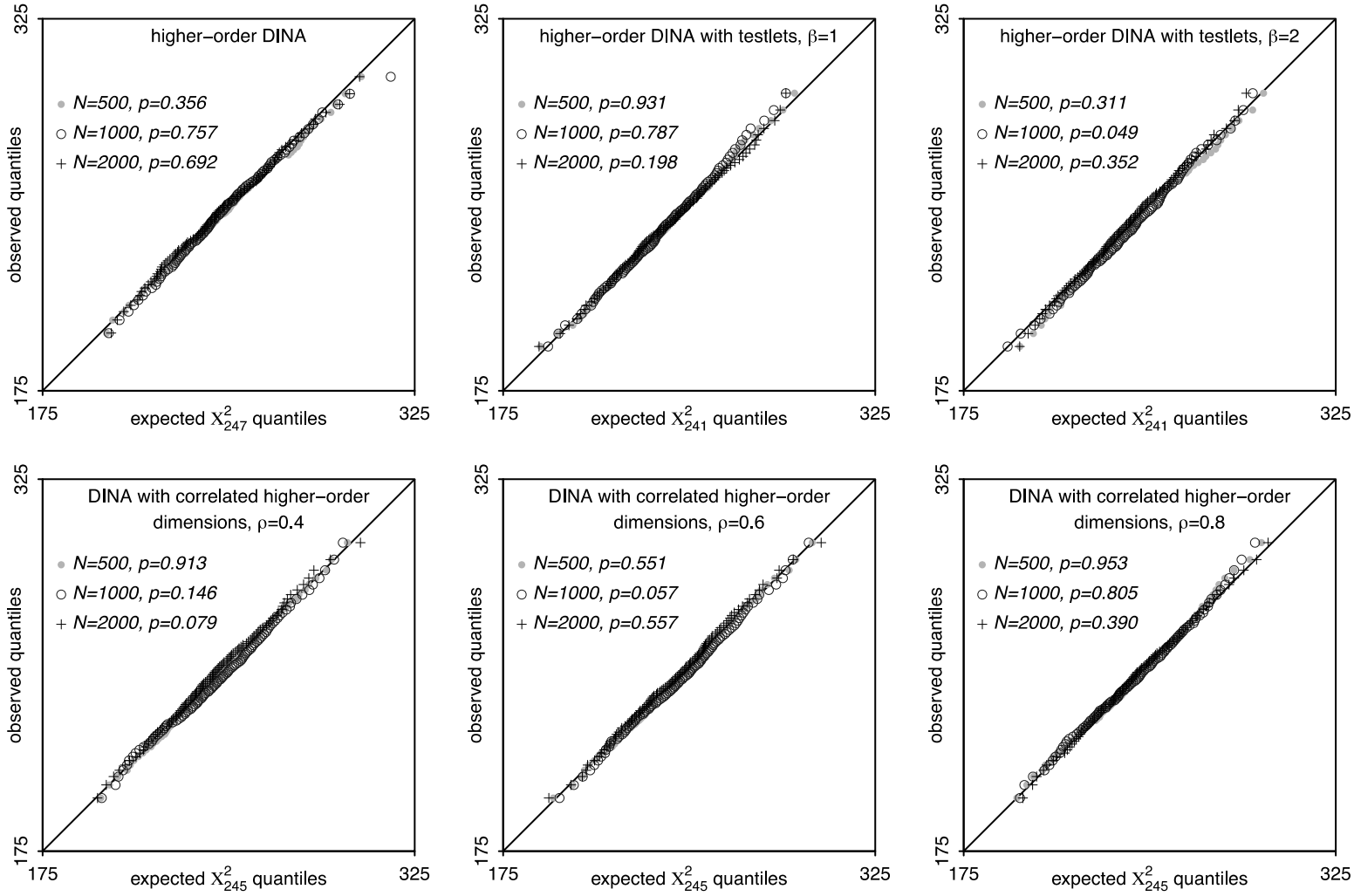

higher−order DINA
N=500, p=0.356
N=1000, p=0.757
N=2000, p=0.692
higher−order DINA with testlets, β=1
N=500, p=0.931
N=1000, p=0.787
N=2000, p=0.198
higher−order DINA with testlets, β=2
N=500, p=0.311
N=1000, p=0.049
N=2000, p=0.352
DINA with correlated higher−order dimensions, ρ=0.4
N=500, p=0.913
N=1000, p=0.146
N=2000, p=0.079
DINA with correlated higher−order dimensions, ρ=0.6
N=500, p=0.551
N=1000, p=0.057
N=2000, p=0.557
DINA with correlated higher−order dimensions, ρ=0.8
N=500, p=0.953
N=1000, p=0.805
N=2000, p=0.390
observed quantiles
expected X^2_{247} quantiles
expected X^2_{241} quantiles
expected X^2_{245} quantiles
175
325

Figure 4

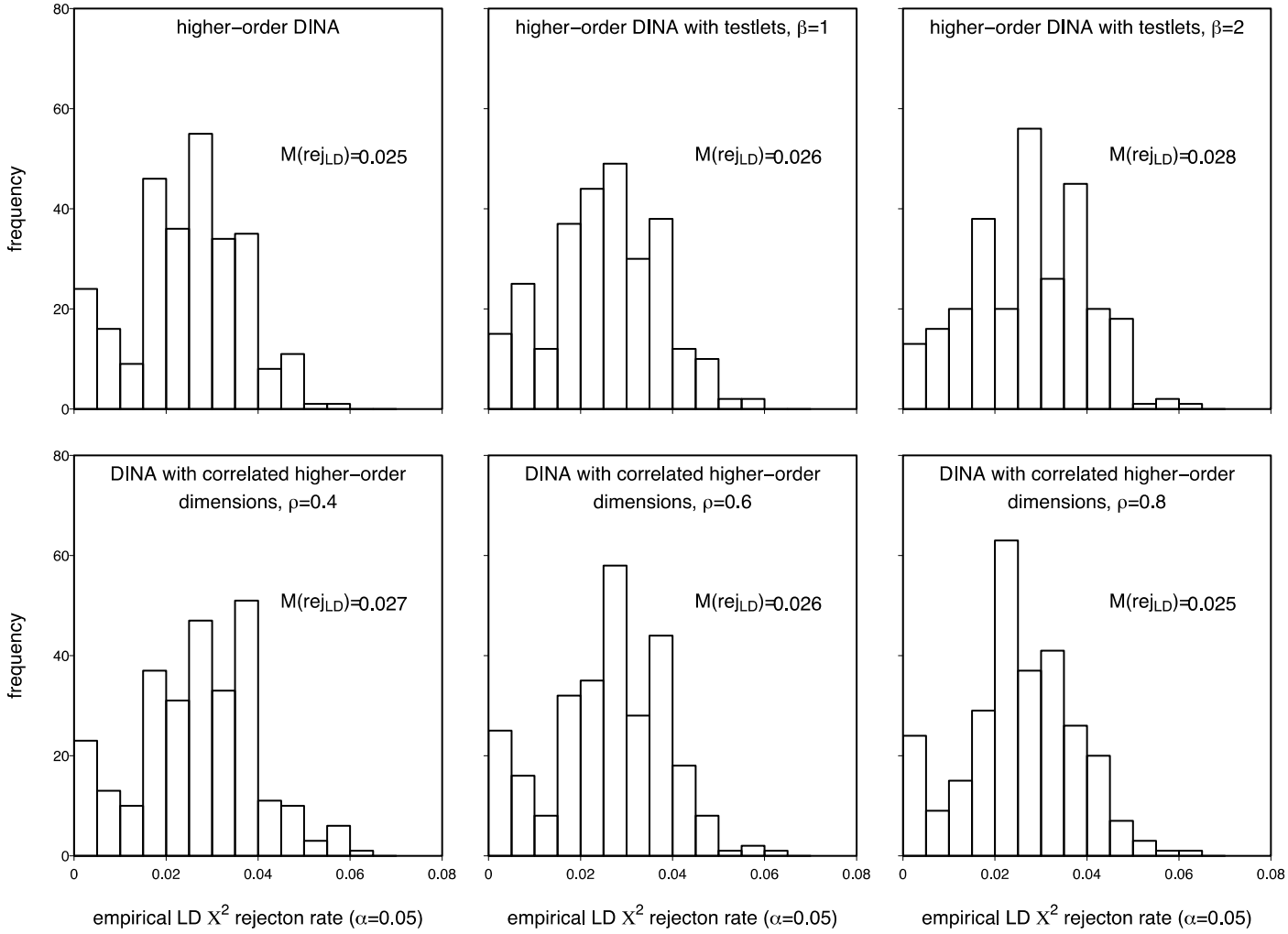

higher−order DINA
M(rej_LD)=0.025
higher−order DINA with testlets, β=1
M(rej_LD)=0.026
higher−order DINA with testlets, β=2
M(rej_LD)=0.028
DINA with correlated higher−order dimensions, ρ=0.4
M(rej_LD)=0.027
DINA with correlated higher−order dimensions, ρ=0.6
M(rej_LD)=0.026
DINA with correlated higher−order dimensions, ρ=0.8
M(rej_LD)=0.025
frequency
empirical LD X2 rejecton rate (α=0.05)
0
20
40
60
80
0.02
0.04
0.06
0.08

Figure 5

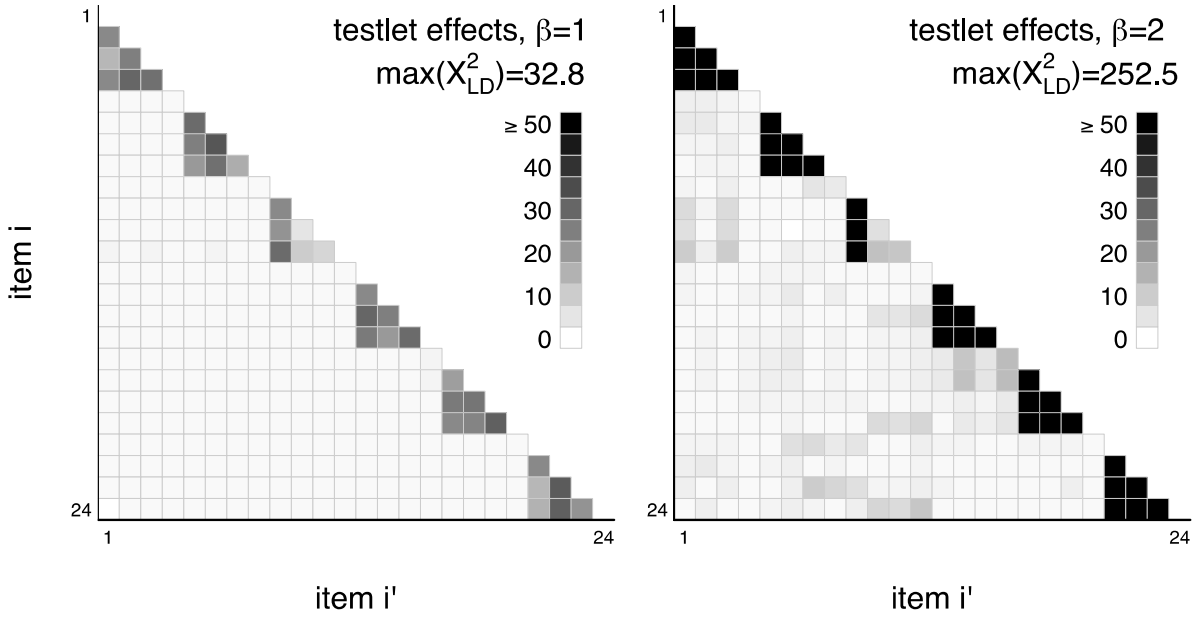

testlet effects, β=1
max(X²LD)=32.8
testlet effects, β=2
max(X²LD)=252.5
≥ 50
40
30
20
10
0
item i
item i'
1
24

Figure 6

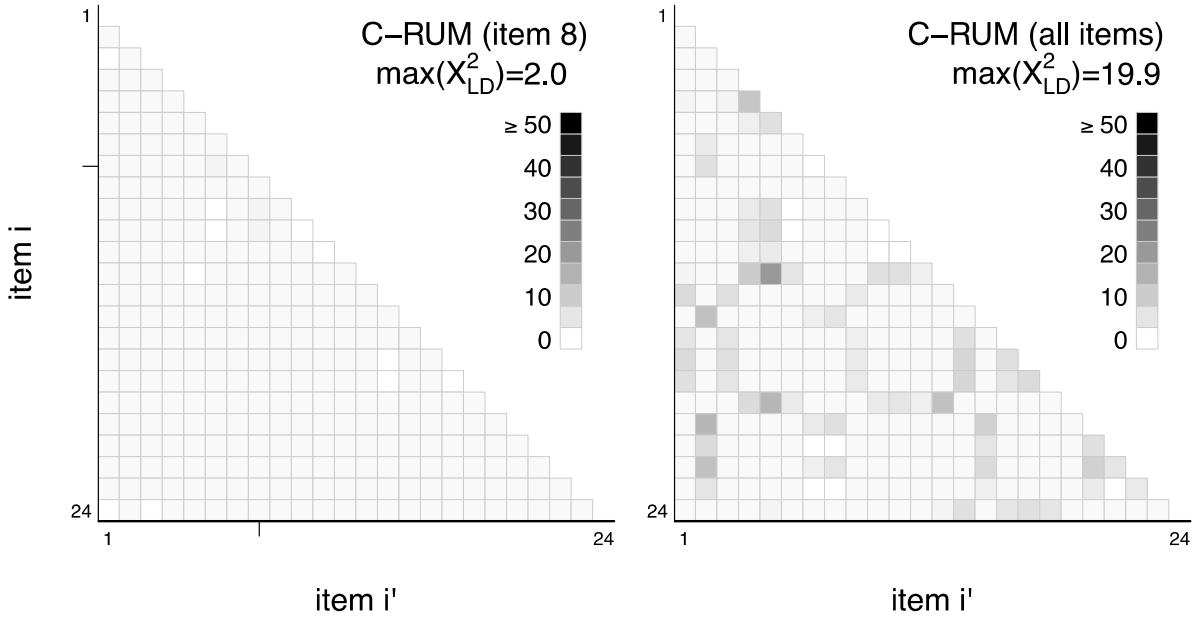

C–RUM (item 8)
max(X²LD)=2.0
C–RUM (all items)
max(X²LD)=19.9
≥ 50
40
30
20
10
0
item i
item i'
1
24

Figure 7

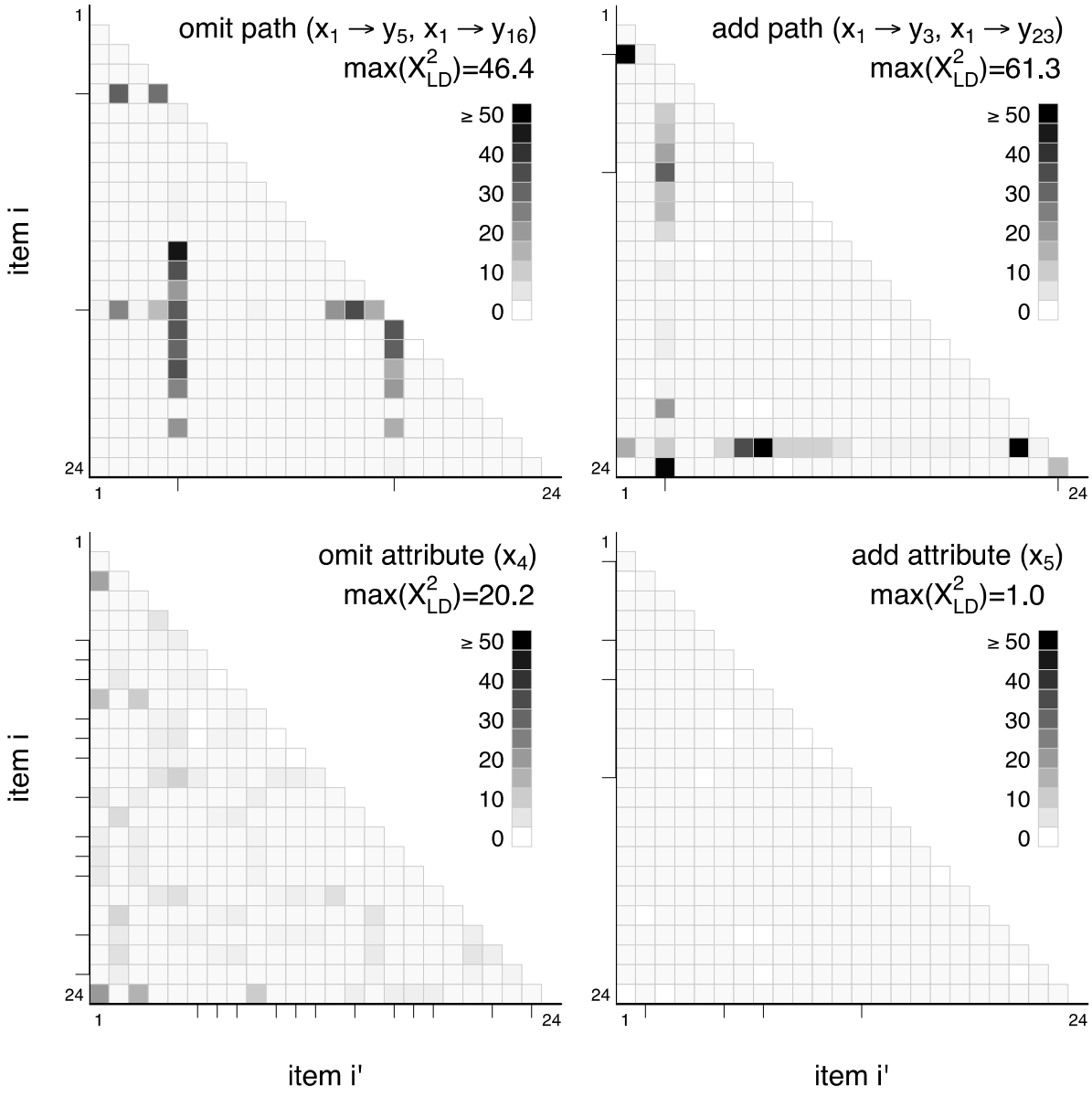
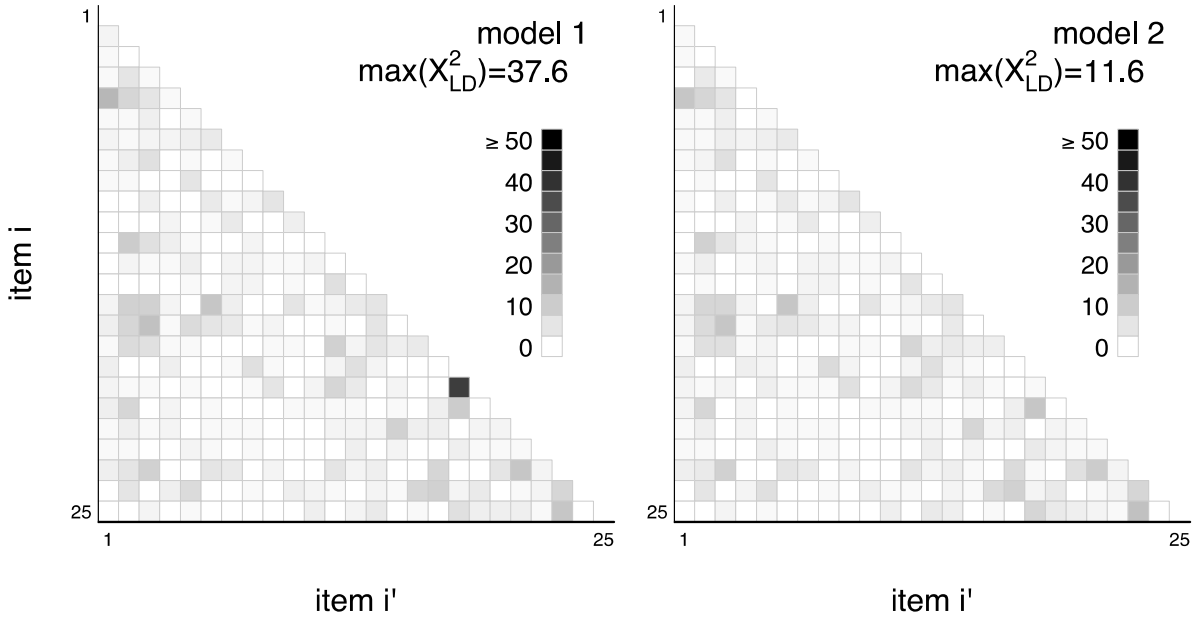

omit path ($x_1 \rightarrow y_5$, $x_1 \rightarrow y_{16}$)
$\max(X^2_{LD})$=46.4
add path ($x_1 \rightarrow y_3$, $x_1 \rightarrow y_{23}$)
$\max(X^2_{LD})$=61.3
omit attribute (x_4)
$\max(X^2_{LD})$=20.2
add attribute (x_5)
$\max(X^2_{LD})$=1.0
≥ 50
40
30
20
10
0
item i
item i'
1
24

Figure 8


model 1
max(X²LD)=37.6
≥ 50
40
30
20
10
0
1
25
item i
item i'
model 2
max(X²LD)=11.6
≥ 50
40
30
20
10
0
1
25
item i'